### owens - 09 / 693213

Jan Delaval Page 1 Reference Librarian Biotechnology & Chemical Library CM1 1E07 – 703-308-4498 jan.delaval@uspto.gov

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### => d l146 bib abs hitrn tot

L146 ANSWER 1 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 2001:781459 HCAPLUS

DN 135:335173

TI Cyclodextrin polymer compositions as drug carriers

IN Kosak, Kenneth M.

PA USA

SO U.S. Pat. Appl. Publ., 28 pp., Cont.-in-part of U.S. 6,048,736. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 2

	PA:	rent	NO.		KII	ND	DATE			A.	PPLI	CATI	N NC	ο.	DATE				
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	WO	1999	-US3	0820	A:	2	1999	1227											
	US	1998	-679	21	В	2	1998	0429	<	_								,	

AB This invention discloses compns. of cyclodextrin polymers for carrying drugs and other active agents. Compns. are also disclosed of cyclodextrin polymer carriers that release drugs under controlled conditions. The invention also discloses compns. of cyclodextrin polymer carriers that are coupled to biorecognition mols. for targeting the delivery of drugs to their site of action. The advantages of the water-sol. cyclodextrin polymer carrier are: drugs can be used based on efficacy without soly. or conjugation requirements; drugs can be delivered as macromols. and released within the cell; drugs can be targeted by coupling the carrier to biorecognition mols.; prepn. methods are independent of the drug to facilitate multiple drug therapies. Thus, a cyclodextrin polymer was

prepd. by the reaction of .beta.-cyclodextrin with 1,4-butanediol diglycidyl ether and 2-aminoanthracene was incorporated into the polymer. ΙT 315-30-0, Allopurinol RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (cyclodextrin polymer compns. as drug carriers) L146 ANSWER 2 OF 25 HCAPLUS COPYRIGHT 2002 ACS 2000:754456 HCAPLUS AN DN 133:306344 Targeted mutagenesis in living cells using modified ΤI oligonucleotides Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall, IN Alexander A. PA Epoch Pharmaceuticals, Inc., USA SO U.S., 19 pp., Cont.-in-part of U.S. 5,849,482. CODEN: USXXAM DT Patent LA English FAN. CNT 8 PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_ \_\_\_\_\_ \_\_\_\_\_ -----US 6136601 Α 20001024 US 1997-827117 19970326 PΙ US 5849482 Α 19981215 US 1995-485611 19950607 <--PRAI US 1991-748138 19910821 В1 US 1994-178733 В2 19940107 US 1995-485611 A2 19950607 US 1988-250474 B2 19880928 <--US 1989-353857 В1 19890518 US 1993-11482 В2 19930126 US 1993-49807 В1 19930420 US 1994-226949 A2 19940627 US 1994-334490 Α 19941104 AΒ A method for introducing a site-specific mutation into a target polynucleotide sequence is presented. The method involves the use of an oligonucleotide capable of binding to the target sequence, either by triplex formation (mediated by Hoogsteen, reverse Hoogsteen or equiv. base pairing) or by Watson/Crick base pairing (in the presence of a recombinase enzyme). The oligonucleotide of the invention is modified by the covalent attachment of one or more electrophilic groups. When a modified oligonucleotide is bound to its target sequence, the electrophilic group is able to interact with a nearby nucleotide in the target sequence, causing a modification to the nucleotide that results in a change in nucleotide sequence. Compns. used in the practice of the method are also disclosed. IT 237059-49-3D, oligonucleotides contg. RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (targeted mutagenesis in living cells using modified oligonucleotides) THERE ARE 133 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 133 ALL CITATIONS AVAILABLE IN THE RE FORMAT L146 ANSWER 3 OF 25 HCAPLUS COPYRIGHT 2002 ACS AN 2000:238403 HCAPLUS DN 132:270079 Cyclodextrin polymers for carrying and releasing drugs TI ΙN

TI Cyclodextrin polymers for carrying and releasing drugs
IN Kosak, Kenneth M.
PA USA
SO U.S., 19 pp., Cont.-in-part of U. S. Ser. No. 67,921, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2
PATENT NO. KIND DATE APPLICATION NO. DATE

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     US 6048736
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                            20010913
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                                                           20010410 <--
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                            19981230
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     WO 1999-US30820
                      W
                           19991227
AB
     This invention discloses methods for prepg. compns. of cyclodextrin
     polymers for carrying drugs and other active agents. Methods are also
     disclosed for prepg. cyclodextrin polymer carriers that release drugs
     under controlled conditions. The invention also discloses methods for
    prepq. compns. of cyclodextrin polymer carriers that are coupled to
    biorecognition mols. for targeting the delivery of drugs to their site of
             The advantages of the water sol. (or colloidal) cyclodextrin
    polymer carrier are: (1) drugs can be used that are designed for efficacy
    without conjugation requirements, (2) it will allow the use of drugs
     designed solely for efficacy without regard for soly., (3) unmodified
     drugs can be delivered as macromols. and released within the cell, (4)
     drugs can be targeted by coupling the carrier to biorecognition mols., (5)
     synthesis methods are independent of the drug to facilitate multiple drug
     therapies. .beta.-Cyclodextrin was crosslinked while complexed
    with anthracene at a molar ratio of 4:1. Chloroform extn. did not remove
     the anthracene, since it was completely entrapped within the cyclodextrin.
IT
     315-30-0, Allopurinol
    RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (cyclodextrin polymers for carrying and releasing drugs)
             THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
L146 ANSWER 4 OF 25 HCAPLUS COPYRIGHT 2002 ACS
AN
    1999:659532 HCAPLUS
    131:296189
DN
ΤI
    Oligonucleotides containing pyrazolo[3,4-d]pyrimidines for
    hybridization and mismatch discrimination
IN
    Meyer, Rich B., Jr.; Afonina, Irina A.; Kutyavin, Igor V.
PA
    Epoch Pharmaceuticals, Inc., USA
    PCT Int. Appl., 51 pp.
SO
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                     KIND DATE
                                         APPLICATION NO. DATE
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                      A1
                           19991025
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                                                           19990405 <--
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    JP 2002510507
                      T2
                            20020409
                                          JP 2000-542486 19990405 <--
PRAI US 1998-54830
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                           19980403
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    WO 1999-US7492
                      W
                           19990405
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Oligonucleotides in which one or more purine residues are
AΒ
     substituted by pyrazolo[3,4-d]pyrimidines exhibit improved hybridization
     properties. Oligonucleotides contg. pyrazolo[3,4-d]pyrimidine
     base analogs have higher melting temps. than unsubstituted
     oligonucleotides of identical sequence. Thus, in assays involving
     hybridization of an oligonucleotide probe to a target
     polynucleotide sequence, higher signals are obtained. In addn.,
     mismatch discrimination is enhanced when pyrazolo[3,4-d]pyrimidine-contg.
     oligonucleotides are used as hybridization probes, making them
     useful as probes and primers for hybridization, amplification and
     sequencing procedures, particularly those in which single- or multiple-
     nucleotide mismatch discrimination is required.
ΙT
     271-80-7D, 1H-Pyrazolo[3,4-d]pyrimidine, derivs. 315-30-0
     2380-63-4, 1H-Pyrazolo[3,4-d]pyrimidin-4-amine 2537-04-4
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
     BIOL (Biological study); OCCU (Occurrence)
        (oligonucleotides contg. pyrazolo[3,4-d]pyrimidines for
        hybridization and mismatch discrimination)
RE.CNT
             THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
L146 ANSWER 5 OF 25 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     1999:659404 HCAPLUS
DN
     131:282379
ΤI
     Hybridization and mismatch discrimination using oligonucleotides
     conjugated to minor groove binders
IN
     Hedgpeth, Joel; Afonina, Irina A.; Kutyavin, Igor V.; Lukhtanov, Eugeny
    A.; Belousov, Evgeniy S.; Meyer, Rich B., Jr.
PA
     Epoch Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 95 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 3
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                                                            DATE
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                      A2
                            19991014
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    WO 9951621
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                           20011017
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             IE, FI
PRAI US 1998-54832
                      Α
                            19980403
                                     <--
     US 1995-415370
                      A2
                            19950403
                                     <--
     WO 1999-US7487
                      W
                            19990405
AΒ
     Conjugates between a minor groove binding mol., such as the trimer of
     1,2-dihydro-(3 H)-pyrrolo[3,2-e]indole-7-carboxylate (CDPI3), and an
     oligonucleotide form unusually stable hybrids with complementary
     target sequences, in which the tethered CDPI3 group resides in the minor
     groove of the duplex. These conjugates can be used as probes and primers.
     Due to their unusually high binding affinity, conjugates as short as
     8-mers can be used as amplification primers with high specificity and
     efficiency. Minor groove binder (MGB) conjugation also increases the
     discriminatory power of short oligonucleotides, providing
     enhanced detection of nucleotide sequence mismatches by short
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oligonucleotides. The MGB-conjugated probes and primers described herein facilitate various analytic and diagnostic procedures, such as

amplification reactions, PCR, detection of single-nucleotide

polymorphisms, gene hunting, differential display, **fluorescence** energy transfer, hydrolyzable probe assays and others; by allowing the use of shorter **oligonucleotides**, which have higher specificity and better discriminatory power.

IT 2380-63-4, 4-Amino-1H-pyrazolo[3,4-d]pyrimidine 2465-59-0 2537-04-4

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(oligonucleotides conjugates contg.; hybridization and mismatch discrimination using oligonucleotides conjugated to minor groove binders)

L146 ANSWER 6 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:505631 HCAPLUS

DN 131:154471

TI Targeted mutagenesis in living cells using modified oligonucleotides

- IN Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall, Alexander A.
- PA Epoch Pharmaceuticals, Inc., USA
- SO U.S., 20 pp. CODEN: USXXAM
- DT Patent
- LA English

FAN. CNT 8

FAN.CNI 8									
	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE.			
			10000010		US 1997-827116	19970326			
Ρ.	I US 5935830	A	19990810						
	US 5849482	Α	19981215		US 1995-485611	19950607 <			
	CA 2223584	AA	19961219		CA 1996-2223584	19960607			
P	RAI US 1995-485611	A2	19950607						
	US 1988-250474	B2	19880928	<					
	US 1989-353857	В1	19890518						
	US 1991-748138	B1	19910821						
	US 1993-11482	B2	19930126						
	US 1993-49807	В1	19930420						
	US 1994-178733	B2	19940107						
	US 1994-226949	A2	19940627						
	US 1994-334490	A	19941104						

- A method for introducing a site-specific mutation into a target AB polynucleotide sequence is presented. The method involves the use of an oligonucleotide capable of binding to the target sequence, either by triplex formation (mediated by Hoogsteen, reverse Hoogsteen or equiv. base pairing) or by Watson/Crick base pairing (in the presence of a recombinase enzyme). The oligonucleotide of the invention is modified by the covalent attachment of one or more electrophilic groups. When a modified oligonucleotide is bound to its target sequence, the electrophilic group is able to interact with a nearby nucleotide in the target sequence, causing a modification to the nucleotide that results in a change in nucleotide sequence. Compns. used in the practice of the method are disclosed. disclosed are arm-leaving group structure having the formula -A-L such as (CH2)qY(CH2)mL, (CH2)qNHCO(CH2)m(X)n'N(R1)(CH2)pL, or (CH2)q'O(CH2)q''NHCO(CH2)m(X)n'N(R1)(CH2)pL (q=0-8, q'=1-7; Y=NH2, OH, SH,COOH, C.ident.CH; X= (Cl, Br, lower alkyl, lower alkoxy-substituted) Ph; n'=0, 1; p= 1-6; R1=H, lower alkyl, or (CH2)pL; L=Cl, Br, I, SO2R2, S+R3; R3,R4=C1-6 alkyl, aryl, heteroaryl, or R3 and R4 form a C1-6-alkylene bridge).
- IT 237059-49-3D, oligonucleotides contg.
  - RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (targeted mutagenesis in living cells using modified oligonucleotides)
- RE.CNT 155 THERE ARE 155 CITED REFERENCES AVAILABLE FOR THIS RECORD

### ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L146 ANSWER 7 OF 25 HCAPLUS COPYRIGHT 2002 ACS
    1998:612101 HCAPLUS
AN
    129:239906
DN
ΤI
    DNA glycosylase inhibitors and their therapeutic uses
ΙN
    Verdine, Gregory L.; Deng, Li
    President and Fellows of Harvard College, USA
PA
SO
    PCT Int. Appl., 78 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
                 KIND DATE
    PATENT NO.
                                       APPLICATION NO. DATE
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    WO 9839334
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PI
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        RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
    US 6369237
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                                         US 1997-812653 19970307
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    WO 1998-US4604
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OS
    MARPAT 129:239906
    The present invention pertains to novel inhibitors of DNA glycosylases.
AΒ
    The invention is based at least in part on the observation that specific
    substituted pyrrolidines, and analogs thereof, are capable of specifically
    inhibiting DNA glycosylases, e.g., as transition state analogs, and
    consequently are useful for modulation of DNA repair. A stereoselective,
    general, and practical synthetic route is developed for these inhibitors.
    An adenine-contq. inhibitor binds adenine glycosylase MutY specifically in
    a strength that surpassed the best inhibitor previously reported for any
    glycosylase. Such compds. can, for example, be used for treating subjects
    having a disorder assocd. with excessive cell proliferation, such as in
    the treatment of various cancers. Furthermore, these glycosylase
    inhibitors can be used as antibacterial, antiviral, and antifungal agents.
    271-80-7DP, 1H-Pyrazolo[3,4-d]pyrimidine, nucleotide
ΙT
    derivs. contg. 315-30-0DP, nucleotide derivs. contg.
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
       (DNA glycosylase inhibitors and their therapeutic uses)
L146 ANSWER 8 OF 25 HCAPLUS COPYRIGHT 2002 ACS
    1998:550433 HCAPLUS
AN
DN
    129:185075
    Targeted modification of the ccr-5 gene with crosslinking
TI
    triplex-forming oligonucleotides
ΙN
    Meyer, Rich B., Jr.; Kutyavin, Igor V.
    Epoch Pharmaceuticals, Inc., USA
PA
SO
    PCT Int. Appl., 34 pp.
    CODEN: PIXXD2
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    Patent
LA
    English
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    WO 1998-US2314
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AB
     Claimed here are oligonucleotides capable of forming
     triple-stranded complexes with the CCR-5 chemokine receptor gene,
     complexing with it via crosslinking. The
     oligonucleotides bear alkylating crosslinking groups,
     capable of causing targeted modification of the CCR-5 gene. Such
     modifications can impair the ability of the CCR-5 gene product to serve as
     a co-receptor for human immunodeficiency viruses.
IT
     2537-04-4
     RL: BPR (Biological process); BSU (Biological study, unclassified); BUU
     (Biological use, unclassified); BIOL (Biological study); PROC (Process);
        (ppG modified base; targeted modification of ccr-5 gene with
        crosslinking triplex-forming oligonucleotides)
L146 ANSWER 9 OF 25 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     1997:148844 HCAPLUS
DN
     126:153646
     Oligonucleotide derivs. preparation for target nucleic
ΤI
     acid alkylation and crosslinking, gene mapping, and gene therapy
ΙN
     Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall,
     Alexander A.; Petrie, Charles R.; Tabone, John C.;
     Hurst, Gerald D.
PA
     Microprobe Corporation, USA
SO
     PCT Int. Appl., 91 pp.
     CODEN: PIXXD2
DT
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     English
LA
FAN.CNT 8
                            DATE
                                           APPLICATION NO. DATE
     PATENT NO.
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             MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT,
             UA, UG
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
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                            19940107
     US 1994-226949
                       Α2
                            19940627
     US 1994-334490
                            19941104
                       Α
     WO 1996-US9551
                       W
                            19960607
     Oligonucleotide derivs. (ODNs) include a sequence that is
AB
     complementary to a target sequence in single-stranded RNA, or single- or
     double-stranded DNA, and an alkylating function which after hybridization
```

alkylates the target sequence. ODNs adapted for alkylating

single-stranded RNA, such as mRNA, are complementary to the target sequence in the Watson Crick sense. ODNs adapted for alkylating double-stranded DNA have at least two alkylating functions and are

complementary to the target sequence in the Hoogsteen or reverse Hoogsteen sense. With these ODNs both strands of the target sequence are alkylated. A third class of ODNs have at least approx. 26 nucleotide units in a continuous sequence which are complementary to the target sequence of double-stranded DNA, and the alkylating function is covalently attached to a nucleotide unit in the continuous sequence. Alkylation or crosslinking with this class of ODNs occurs in the presence of a recombinase enzyme.

IT 129357-70-6P 129357-75-1P 129357-76-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction; oligonucleotide derivs. prepn. for target nucleic acid alkylation and crosslinking, gene mapping, and gene therapy)

IT 137823-47-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn.; oligonucleotide derivs. prepn. for target
 nucleic acid alkylation and crosslinking, gene
 mapping, and gene therapy)

L146 ANSWER 10 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1990:532717 HCAPLUS

DN 113:132717

TI Preparation of pyrazolo[3,4-d]pyrimidine derivatives as intermediates for diagnostic oligonucleotides

IN Petrie, Charles R.; Meyer, Rich B.

PA Microprobe Corp., USA

SO PCT Int. Appl., 41 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 8

ran. Cni o									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
PΙ	WO 9003370	A1	19900405	WO 1989-US4184	19890926 <				
	W: JP								
	RW: AT, BE,	CH, DE	, FR, GB,	IT, LU, NL, SE					
	CA 1338379	A1	19960611	CA 1989-613651	19890927 <				
	US 5824796	A	19981020	US 1994-334490	19941104 <				
PRAI	US 1988-250474	Α	19880928	<					
	US 1989-353857	B1	19890518						
	US 1993-49807	В1	19930420						
os	MARPAT 113:1327	17							
GT									

AB The title compds. [I; R1 = H, sugar moiety optionally substituted at its 3' or 5' position with mono-, di-, or triphosphate or a reactive group suitable for nucleotide bond formation; provided that when R3 = H, R1 .noteq. H; R3 = H, W(X)nA; W, X = chem. linker arm; A = intercalator, electrophilic crosslinker, reporter group; R4, R6 = H, OH, SH, alkylthio, NH2, NH(CH2)tNH2; n = 0,1; t = 0-12] were prepd. by (1) reaction of 5-aminopyrazole-4-carbonitriles (II; R = cyano; R1, R3 = as above) with a dialkoxymethyl carboxylate

followed by reaction with NH3 to give I (R4 = NH2), (2) reaction of II (R= CONH2; R1, R3 = as above) with a dialkoxymethyl carboxylate to give I (R4 = OH), or (3) reaction of II (R = cyano, CONH2; R1, R3 = as above) with an alkyl xanthate salt followed by an alkyl halide and oxidn. An oligonucleotide sequence contg. .gtoreq.1 of labeled I (R1 = sugar moiety as described above), particularly labeled with biotin, is used as DNA hybridization probe and as a kit for identifying target DNA sequence comprising the above labeled oligonucleotide complementary to the target DNA, a denaturation reagent, and a hybridization reaction mixt. (no data). Thus, 5-amino-1-(2-deoxy-3,5-di-0-toluoyl-.beta.-D-erythropentofuranosyl)-3-[(5tritylamino)pentyl]pyrazole-4-carbonitrile was heated 5 h at 80-90.degree. with AcOCH2(OEt)2 and the intermediate syrup was treated 2 days at room temp. with methanolic NH3 to give 77% I [R1 = Q, R2 = R6 = H, R3 =(CH2)5NHCPh3, R4 = NH2]. This was phosphorylated by reaction with POCl3 in (MeO) 3PO followed by hydrolysis with 0.1 M NH4HCO3 to give I [R1 = Q,R2 = (HO) 2P(O), R3 = (CH2) 5NHCPh3, R4 = NH2, R6 = H] which was hydrogenolyzed over Pd(OH)2/C in cyclohexadiene and then acylated with N-hydroxysuccinimidyl 6-biotinamidocaproate in DMF contg. Et3N to give I [R1 = Q, R2 = (HO)2P(O), R3 = 5-[(6-biotinamido)hexamido]pentyl, R4 = NH2,R6 = H].

IT 129357-75-1P 129357-76-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of biotin-labeled deoxyribofuranosylpyrazolopyrimidine nucleotide)

IT 129357-70-6P 129357-71-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for **oligonucleotide** hybridization probes)

L146 ANSWER 11 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1989:173656 HCAPLUS

DN 110:173656

TI Synthesis and cytotoxic activity of 4,6-diaminopyrazolo[3,4-d]pyrimidine riboside and its 3-carbamoyl derivative

AU Garaeva, L. D.; Korbukh, I. A.; Dobrynin, Ya. V.; Nikolaeva, T. G.; Preobrazhenskaya, M. N.

CS VONTs, Moscow, USSR

SO Khim.-Farm. Zh. (1988), 22(7), 798-802 CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

OS CASREACT 110:173656

GI

Treating nucleoside I (R = CN, R1 = .beta.-D-ribofuranosyl) with aq. NH3 and H2O2 gave 76% I (R = CONH2) which underwent amination by methanolic NH3 in an ampul to give 70% amino deriv. II (R2 = MeS) whose oxidn. by m-ClC6H4C(O)OOH gave 90% sulfone II (R2 = MeSO2). Treatment of the latter with NH3(l) in an ampul eliminated the methylsulfonyl group to give 70% diamino deriv. II (R2 = NH2). The most cytotoxic of the groups were the 4,6-bis(methylmercapto)- and diaminonucleosides contg.

```
a carbamoyl group.
ΙT
     119952-34-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and amination of)
     70421-30-6P 116019-28-4P 119952-37-3P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and cytotoxic activity of)
ΙT
     69259-11-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and oxidative ammonolysis of)
TT
     74525-93-2P 119952-35-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and oxidn. to sulfone)
TΤ
     73236-32-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
L146 ANSWER 12 OF 25 HCAPLUS COPYRIGHT 2002 ACS
     1988:132231 HCAPLUS
ΑN
DN
     108:132231
    A new method for synthesizing acyclonucleosides
TΙ
     Lazrek, H. B.; Taha, M. L.; Barascut, J. L.; Imbach, J. L.
ΑU
CS
     Dep. Chim., Fac. Sci., Marrakech, Morocco
SO
     Nucleosides Nucleotides (1987), 6(1-2), 379-80
     CODEN: NUNUD5; ISSN: 0732-8311
DT
     Journal
LA
     English
AΒ
    A report from the 7th round table symposium held in 1986. A new
     series of acyclonucleoside analogs of allopurinol, where the
     ribose moiety is replaced by the (2-hydroxyethoxy)methyl group
    was prepd. using phase-transfer catalysis.
ΙT
     315-30-0DP, Allopurinol, acyclonucleoside analogs
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
L146 ANSWER 13 OF 25 HCAPLUS COPYRIGHT 2002 ACS
     1987:214304 HCAPLUS
AN
     106:214304
DN
    Labeled (poly) nucleotides
ΤI
     Sugimoto, Nobutaka; Sato, Toyoki
ΙN
PΑ
     Yuki Gosei Kogyo Co., Ltd., Japan
     Jpn. Kokai Tokkyo Koho, 6 pp.
SO
     CODEN: JKXXAF
DT
     Patent
LA
     Japanese
FAN.CNT 1
                                         APPLICATION NO. DATE
     PATENT NO.
                     KIND DATE
                                          ______
                                         JP 1984-231847 19841101 <--
PΙ
     JP 61109797
                     A2 19860528
OS
    CASREACT 106:214304
GΙ
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- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- Purine base residues I (R, R1 = H, OH, NH2; X, X1, X2 = C, N; R2 = fluorescence labeled compds. (except 7-deazapurine) linked to (poly)ribonucleotides and (poly) deoxyribonucleotides, useful for identification and extn. of target genes (no data), were prepd. Thus, malononitrile was treated with hydrazine to give 3-(cyanomethyl)-4-cyano-5-aminopyrazole.

Cyclocondensation of this with HCHO and Raney Ni redn. of the resulting 4-amino-3-(cyanomethyl)pyrazolo[3,4-d]pyrimidine gave a purine analog II (R = H). Glycosidation of protected II (R = Ac) with 3,5-di-O-acetyl-beta.-D-deoxyribosyl chloride gave, after deacetylation, a nucleoside III. Then a nuleoside deriv. IV (a deriv. of III) was condensed with C-C-T (C = cytosine; T = thymine) to give, after deprotection, Q-C-C-T-Q-C-C-T-T (Z = nucleotide whose base residue after deprotection is II) (V). Then I was fluoroescence-labeled by dansyl chloride in acetone.

IT 38340-27-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and Raney Nickel redn. of)

IT 107296-14-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and benzoylation, dimethoxytritylation, and phosphorylation of)

IT 46153-15-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and protection of)

L146 ANSWER 14 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1986:221087 HCAPLUS

DN 104:221087

TI Specificity of adenine binding to lima bean lectin

- AU Roberts, David D.; Arjunan, Palanisamy; Townsend, Leroy B.; Goldstein, Irwin J.
- CS Dep. Biol. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA
- SO Phytochemistry (1986), 25(3), 589-93 CODEN: PYTCAS; ISSN: 0031-9422

DT Journal

LA English

- The interactions between lima bean lectin (LBL) and adenine were examd. AB using a series of synthetic purine analogs. Binding was sensitive to modification at most positions of the purine ring, suggesting a high degree of specificity for adenine binding. Methylation of the 6 NH2group to MeNH-, Me2N- and Me3N+-analogs progressively decreased the binding affinity. Compds. lacking the 6 NH2-group were not bound. Methylation of adenine at N1, N3 or N7 also inhibited binding, indicating specific interactions with these ring nitrogens. In contrast to the previous report that N9-substituted adenines, nucleosides and nucleotides were not bound (Roberts, D. D., et al., 1983), 9-methyl- and 9-benzyl-substituted adenines were bound to LBL with high affinity. Substitutions at C-2 and C-8 were tolerated and, in some cases, increased the affinity of binding to LBL. Heterotropic interactions between the adenine and 1,8anilinonaphthalenesulfonate binding sites were also sensitive to modification of the purine ring. 2-Methylthioadenine and 4-aminopyrazolo[3,4-d]pyrimidine showed increased allosteric interaction with 1,8-anilinonaphthalenesulfonate binding, whereas several adenine analogs with a 9-p-nitrobenzyl substituent appeared to be neg. effectors of 1,8-anilinonaphthalenesulfonate binding.
- ·IT 2380-63-4 6826-96-6

RL: BIOL (Biological study) (lima bean lectin binding by)

L146 ANSWER 15 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1985:437693 HCAPLUS

DN 103:37693

- TI Synthesis and biological activity of 6-azacadeguomycin and certain 3,4,6-trisubstituted pyrazolo[3,4-d]pyrimidine ribonucleosides
- AU Petrie, Charles R., III; Cottam, Howard B.; McKernan, Patricia A.; Robins, Roland K.; Revankar, Ganapathi R.
- CS Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA
- SO J. Med. Chem. (1985), 28(8), 1010-16

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal LA English

OS CASREACT 103:37693

GI

AΒ High-temp. glycosylation of 3,6-dibromoallopurinol with 1-O-acetyl-2,3,5-tri-O-benzoyl-D-ribofuranose in the presence of BF3.cntdot.OEt2, followed by ammonolysis, provided nucleoside I. Similar glycosylation of either 3-bromo-4(5H)-oxopyrazolo[3,4-d]pyrimidin-6-yl Me sulfoxide or 6-amino-3-bromopyrazolo[3,4-d]pyrimidin-4(5H)-one, and subsequent ammonolysis, also gave I. Application of this glycosylation procedure to 6-(methylthio)-4(5H)-oxopyrazolo[3,4d]pyrimidine-3-carboxamide gave the corresponding N-1 glycosyl deriv. II (R = Bz, R1 = SMe, R2 = CONH2)(III). Dethiation and debenzoylation of III provided an alternate route to the recently reported 3carbamoylallopurinol ribonucleoside. Oxidn. of III and subsequent ammonolysis afforded 6-amino-1-.beta.-D-ribofuranosyl-4(5H)oxopyrazolo[3,4-d]pyrimidine-3-carboxamide (IV) which on alk. treatment gave 6-azacadeguomycin II (R = H, R1 = NH2, R2 = CO2H). Acetylation of IV, followed by dehydration with phosgene, provided the versatile intermediate II (R = Ac, R1 = NH2, R2 = cyano) (V). Deacetylation of V gave 6-amino-1-.beta.-D-ribofuranosyl-4(5H)-oxopyrazolo[3,4-d]pyrimidine-3carbonitrile. Reaction of V with H2S gave II (R = H, R1 = NH2, R2 = CSNH2). All of these compds. were tested in vitro against certain viruses and tumor cells. Among these compds., the guanosine analogs I and II (R = H, R1 = NH2, R2 = cyano) showed significant activity against measles in vitro and exhibited moderate antitumor activity in vitro against L1210 and P388 leukemia. 6-Azacadeguomycin and all other compds. were inactive against the viruses and tumor cells tested in vitro.

IT 5334-26-9 24521-76-4

RL: RCT (Reactant)

(bromination of)

IT 96555-44-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and acetylation of)

IT 96555-41-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and deblocking of)

IT 96555-37-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and debromination of)

IT 96555-45-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and dehydration of)
96555-46-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and desulfuration or oxidn. of)

IT 96575-36-9P

ΙT

IT 96555-43-0P 96575-35-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and ribosylation of)

IT 85426-74-0P 90914-46-8P 96555-38-3P 96555-48-5P 96555-49-6P 96555-50-9P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

L146 ANSWER 16 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1984:491391 HCAPLUS

DN 101:91391

TI Synthesis and biological activity of certain 3,4-disubstituted pyrazolo[3,4-d]pyrimidine nucleosides

AU Cottam, Howard B.; Petrie, Charles R.; McKernan, Patricia A.; Goebel, Richard J.; Dalley, N. Kent; Davidson, Richard B.; Robins, Roland K.; Revankar, Ganapathi R.

CS Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA

SO J. Med. Chem. (1984), 27(9), 1119-27 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

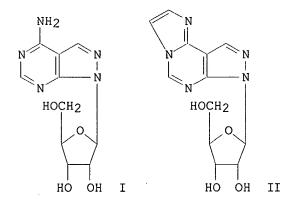
GΙ

AB Several title **ribonucleosides**, e.g., I [R = Br, cyano, SMe, NH2, NHMe, NMe2, CONH2, CSNH2, C(:NH)NH2, C(:NOH)NH2; R1 = H, Bz; Z = O, S], were prepd. I (R = Br, cyano; R1 = Bz; Z = O), obtained by glycosylation of the corresponding heterocycles with 1-O-acetyl-2,3,5-tri-O-benzoyl-D-ribofuranose, were the key intermediates. The structural assignment of I (R = cyano, R1 = H, Z = O) was made by single crystal x-ray anal. All the compds. were tested in vitro against certain viruses, tumor cells, and the parasite Leishmania tropica. I [R = CSNH2, C(:NH)NH2; R1 = H; Z = O] showed significant activity against Para 3 virus and were potent inhibitors of growth of L1210 and P388 leukemia. I (R = cyano, R1 = H, Z = S) showed the most significant broad-spectrum antiviral and antitumor

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activity. I (R = Br, R1 = H, Z = O) was more active than allopurinol
     riboside against L. tropica within human macrophages.
IT
     90914-42-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and amination of, with ammonia)
IT
     90914-37-7P 90914-43-5P 90914-51-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and debenzoylation of)
IT
     90914-31-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and debromination of)
TT
     90914-32-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and desulfuration of)
IT
     90914-30-0P 90914-33-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reactions of)
IT
     16220-07-8P 90914-34-4P 90914-36-6P
     90914-38-8P 90914-39-9P 90914-40-2P
     90914-44-6P 90914-46-8P 90914-47-9P
     90914-48-0P 90914-49-1P 90914-50-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IT
     90914-52-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, attempted)
     5387-84-8 54738-73-7 83255-86-1
ΙT
     RL: RCT (Reactant)
        (ribofuranosylation of)
L146 ANSWER 17 OF 25 HCAPLUS COPYRIGHT 2002 ACS
AN
     1982:7014 HCAPLUS
DN
     96:7014
ΤI
     The nucleosides of substituted pyrazolo(3,4-d)pyrimidines
ΑIJ
     Korbukh, I. A.; Bulychev, Yu. N.; Yakunina, N. G.; Preobrazhenskaya, M. N.
CS
     All-Union Cancer Res. Cent., Moscow, 115478, USSR
     Nucleic Acids Symp. Ser. (1981), 9, 73-5
SO
     CODEN: NACSD8
DΤ
     Journal
LA
     English
     The 1-.beta.-D-ribosides of 4-, 3,4-, 4,6- and 3,4,6-substituted
AB
     pyrazolo[3,4-d]pyrimidines were prepd. by regioselective glycosylation and
     subsequent transformations.
     5418-10-0 6288-89-7 73236-31-4
TΤ
     78710-14-2 80117-79-9
     RL: RCT (Reactant)
        (glycosylation of, with ribofuranose tetraacetate)
     60355-66-0P 73236-32-5P 76690-43-2P
IT
     78710-16-4P 80117-80-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and deacetylation of)
TT
     60355-67-1P 69259-11-6P 74525-92-1P
     78710-19-7P 80117-81-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reactions of)
TΤ
     60355-67-1P 69259-11-6P 74516-76-0P
     74516-77-1P 74516-78-2P 74516-79-3P
     74516-80-6P 74516-81-7P 74516-82-8P
     74516-84-0P 74525-92-1P 74525-93-2P
     74525-95-4P 76690-46-5P 78710-19-7P
     78710-20-0P 78710-21-1P 78710-22-2P
     78710-23-3P 80117-82-4P 80117-83-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
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(prepn. of)

L146 ANSWER 18 OF 25 HCAPLUS COPYRIGHT 2002 ACS 1981:620260 HCAPLUS AN DN 95:220260 ΤI Synthesis of certain fluorescent tricyclic nucleosides derived from pyrazolo[3,4-d]pyrimidine nucleosides Bhat, Ganapati A.; Townsend, Leroy B. ΑU Dep. Med. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA CS J. Chem. Soc., Perkin Trans. 1 (1981), (9), 2387-93 SO CODEN: JCPRB4; ISSN: 0300-922X DΤ Journal LA English



- The prepn. is described of tricyclic nucleosides with a dihydroimidazole, imidazole, triazole, or tetrazole ring fused to the pyrazolopyrimidine ring system in an angular position. E.g., cyclocondensation reaction of the nucleoside I with ClCH2CHO (H2O, NaOAc, pH 4.5, 80.degree., 3 h) gave the imidazo deriv. II (64%). The UV and fluorescence spectra of the tricyclic nucleosides are reported.
- IT **64372-76-5**

GI

RL: PROC (Process)

(cyclization and acetalization of)

IT 3258-05-7

RL: RCT (Reactant)

(cycloamination reactions of, tricyclic nucleosides by)

L146 ANSWER 19 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1981:525862 HCAPLUS

DN 95:125862

- TI Pyrazolopyrimidine nucleosides. 12. Synthesis and biological activity of certain pyrazolo[3,4-d]pyrimidine nucleosides related to adenosine
- AU Bhat, Ganapati A.; Montero, Jean Louis G.; Panzica, Raymond P.; Wotring, Linda L.; Townsend, Leroy B.
- CS Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109, USA
- SO J. Med. Chem. (1981), 24(10), 1165-72 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GΙ

AB Twenty-six title compds., 13 of which were synthesized, were tested for antitumor activity against mouse L1210 leukemia cells both in vitro and in vivo and against P388 leukemia cells in vivo. I [3258-05-7] and II [78586-44-4] showed the greatest inhibition of growth of L1210 cells in vitro, with the activity of II probably resulting from the formation of I by hydrolysis in the aq. medium. Any alteration of the C4-amino substituent of I resulted in a decrease or loss of antitumor activity. Certain substitutions at the C3 position of I resulted in compds. with a better antitumor activity than I. III [55559-56-3] was the most active compd. giving an increase in life-span of 136% (vs. 48% for I) in L1210-bearing mice and having a significant lethal effect on L1210 cells in vitro.

IT 16220-07-8 54524-71-9 55559-50-7 55559-51-8 55559-52-9 55559-53-0 55559-54-1 55559-55-2 55559-56-3 55559-57-4 64372-72-1 64372-77-6

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (antitumor activity of, structure in relation to)

IT 3258-05-7P 60355-67-1P 64372-76-5P

70421-26-0P 78586-40-0DP, derivs. 78586-40-0P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and antitumor activity of, structure in relation to)

IT 64372-69-6

RL: RCT (Reactant)

(redn. and chlorination of)

L146 ANSWER 20 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1981:498198 HCAPLUS

DN 95:98198

TI Synthesis of derivatives of pyrazolo[3,4-d]pyrimidin-3-ylacetic acid and their nucleosides

AU Bulychev, Yu. N.; Korbukh, I. A.; Preobrazhenskaya, M. N.

CS Onkol. Nauchn. Tsentr, Moscow, 115478, USSR

SO Khim. Geterotsikl. Soedin. (1981), (4), 536-45 CODEN: KGSSAQ; ISSN: 0453-8234

DT Journal

LA Russian

GΙ

$$\begin{array}{c|c} & & & \\ & & & \\ \text{MeS} & & & \\ & & & \\ N & & & \\ N & & & \\ N & & & \\ R3 & & & IV \\ \end{array}$$

Pyrazolopyrimidine I (R = R1 = H, n = 1), prepd. in 87% yield from II by cyclocondensation with CS2, hydrolysis, and methylation, were ribosylated by 1,2,3,5-tetra-O-acetyl-.beta.-D-ribofuranose to give I (R = 2,3,5-tri-O-acetyl-.alpha.,.beta.-D-ribofuranosyl, R1 = H, n = 1; R = H, R1 = 2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl, n = 1). Addnl. obtained were 54 and 40% III (R2 = CO2NH4, CN, R3 = .beta.-D-ribofuranosyl) and 20 and 53% IV (R2 = CN, CONH2, R3 = .beta.-D-ribofuranosyl). Treatment of the 6-methylthio derivs. with morpholine and piperidine gave the corresponding amino derivs.

IT 78710-13-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and methylation of)

IT 78710-14-2P 78710-16-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reactions of)

TT 78710-15-3P 78710-17-5P 78710-19-7P 78710-20-0P 78710-21-1P 78710-22-2P

78710-23-3P 78724-02-4P

Ι

III

L146 ANSWER 21 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1979:87798 HCAPLUS

DN 90:87798

TI Nucleosides of pyrazolopyrimidines

AU Blanko, F. F.; Goryunova, O. V.; Bulychev, Yu. N.; Korbukh, I. A.; Preobrazhenskaya, M. N.

CS USSR

SO Novosti Khimii Nukleozidov i Nukleotidov (1978) 30-2 From: Ref. Zh., Khim. 1978, Abstr. No. 18E94

DT Journal

LA Russian

AB Title only translated.

IT 60355-67-1P 69259-11-6P

L146 ANSWER 22 OF 25 HCAPLUS COPYRIGHT 2002 ACS

AN 1975:572354 HCAPLUS

DN 83:172354

- TI Metabolism of allopurinol-6-14C. Lack of incorporation of allopurinol into nucleic acids
- AU Nelson, Donald J.; Elion, Gertrude B.
- CS Wellcome Res. Lab., Research Triangle Park, N. C., USA
- SO Biochem. Pharmacol. (1975), 24(11-12), 1235-7

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CODEN: BCPCA6
DT
     Journal
     English
LA
     Anal. of the radioactive species present in hydrolyzates of RNA from
AΒ
     intestine of rats after administration of 6-14C-labeled
     allopurinol [315-30-0] (50 mg/kg, 2.4 mCi/mmole, i.v.) confirmed
     the lack of incorporation of allopurinol or its metabolites into
     nucleic acids.
ΙT
     315-30-0
     RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
        (metab. of, nucleic acids in relation to)
L146 ANSWER 23 OF 25 HCAPLUS COPYRIGHT 2002 ACS
     1975:171339 HCAPLUS
AN
DN
     82:171339
TI
     Pyrazolopyrimidine nucleosides. VII. Synthesis of certain
     pyrazolo[3,4-d]pyrimidine nucleosides related to the
     nucleoside antibiotics toyocamycin and sangivamycin
ΑU
     Earl, Robert A.; Townsend, Leroy B.
CS
     Dep. Chem., Univ. Utah, Salt Lake City, Utah, USA
SO
     J. Heterocycl. Chem. (1974), 11(6), 1033-9
     CODEN: JHTCAD
\mathsf{D}\mathbf{T}
     Journal
LA
     English
AΒ
     The condensation of 4-acetamido-3-cyanopyrazolo[3,4-d]pyrimidine with
     2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl chloride, which evolved copius
     amts. of HCN, was followed by treatment with NaOMe in MeOH to give Me
     4-amino-1-(.beta.-D-ribofuranosyl)pyrazolo[3,4-d]pyrimidine-3-formimidate
     monohydrate (I). The formimidate function of I was highly reactive and
     was readily converted into the corresponding carboxamidine,
     carboxamidoxime, and carboxamidrazone. Treatment of I with NaHS gave a
     high yield of the thiocarboxamide, which was then converted into
     4-amino-3-cyano-1-(.beta.-D-ribofuranosyl)pyrazolo[3,4-d]pyrimidine. Aq.
     base transformed I into 4-amino-1-(.beta.-D-ribofuranosyl)pyrazolo[3,4-
     d]pyrimidine-3-carboxamide while more vigorous basic hydrolysis gave the
     corresponding carboxylic acid (II) in nearly quant. yield.
     Decarboxylation of II in hot sulfolane gave 68% 4-amino-1-(.beta.-D-
     ribofuranosyl)pyrazolo[3,4-d]pyrimidine which established the site of
     ribosylation and anomeric configuration for all nucleosides
     reported in this investigation.
ΙT
     6826-96-6
     RL: RCT (Reactant)
        (acetylation of)
ΙT
     55559-50-7P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reactivity of)
     3258-05-7P 55559-51-8P 55559-52-9P
ΤT
     55559-53-0P 55559-54-1P 55559-55-2P
     55559-56-3P 55559-57-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
L146 ANSWER 24 OF 25 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     1975:41629 HCAPLUS
DN
     82:41629
     Synthesis of purine nucleotides in human and leukemic cells.
TI
     Interaction of 6-mercaptopurine and allopurinol.
ΑU
     Wilmanns, W.
     Dep. Intern. Med. II, Univ. Clin., Tuebingen, Ger.
CS
     Adv. Exp. Med. Biol. (1974), 41A, 147-58
SO
     CODEN: AEMBAP
DT .
     Journal
LA
     English
```

AB In a study of the effect of 6-mercaptopurine (I) on the tetrahydrofolate-dependent activation of formate (II)-14C in relation to the net de novo synthesis of purine nucleotides in cell-free exts. of normal and leukemic leukocytes the incorporation of II-14C into nucleotides could be detected only if all components necessary for the de novo pathway were added to the incubation mixt. together with the substrates and cofactors of the II-activating system. The purines identified were hypoxanthine and adenine. The activating enzyme, tetrahydrofolate formylase (III), was found in normal and leukemic leukocytes, the highest activities being observed in immature blast cells of acute leukemia. By detn. of the II-14C incorporation, a measurable net de novo synthesis of nucleotides was detected only in immature leukemic cells. If different patients with acute leukemia were studied, the amt. of II-14C incorporation was correlated to the activity of the III. In addn., the rate of II-14C incorporation into nucleotides depended on the concn. of tetrahydrofolate in the incubation mixt. It could be assumed that the rate of de novo synthesis of nucleotides was controlled by the 1st reaction of this pathway (involving phosphoribosylpyrophosphate amidotransferase) and the amt. of N10-formyltetrahydrofolate available for incorporation of activated formyl groups into the C-2 and C-8 positions of the purine ring. Although I in a rather high concn. (1.5 .times. 10-3M) had only a small inhibitory effect on III in the leukemic blast cells of patients with acute leukemia, inhibition of III by I was markedly increased by the addn. of allopurinol (IV), whereas IV alone had no effect. This was explained by the fact that IV, by inhibiting xanthine oxidase, reduced the inactivation of I to 6-thiouric acid. Autoradiog. following the chromatog. sepn. of blast-cell hypoxanthine-14C and IMP-14C, formed by hypoxanthine-guanine phosphoribosyltransferase (V), showed that V was inhibited by I. The I concn. necessary for inhibition of this reaction was about 0.1 of that in the III reaction. As V was also specific for I, the latter was transformed to thioinosinic acid, which was regarded as the metabolically active inhibitor of the de novo synthesis of purine. The addn. of IV affected neither the inhibition of the V by I nor the conversion of I to thioinosinic acid by the same enzyme. It was unlikely that this was due to a lack of xanthine oxidase in the cells investigated. It was concluded that a conversion of I to the monophosphoribonucleotide was not necessary for the inhibition of II activation. Only the inhibitory effect of I on this reaction, which was important for the de novo synthesis of nucleotides, was potentiated by IV. The competition of both substances with xanthine oxidase was assumed to be the biochem. basis for this interaction. Thus, the inactivation of I by oxidn. to thiouric acid could be prevented by IV. The clin. observation of a higher cytotoxic effect of I treatment, if patients received IV at the same time, was explained by these results. 315-30-0

IT

RL: BIOL (Biological study) (leukemia response to, purine nucleotide formation in, mercaptopurine in relation to)

L146 ANSWER 25 OF 25 HCAPLUS COPYRIGHT 2002 ACS

ΑN 1968:417563 HCAPLUS

DN 69:17563

- TΙ Effects of 4-aminopyrazolo(3,4-d)pyrimidine in combination with quanine on nucleic acid and protein synthesis by Ehrlich ascites cells in culture. Biochemical and cytochemical analyses
- ΑŲ Schachtschabel, D. O.; Killander, D.; Zetterberg, A.; McCarthy, R. E.; Foley, G. E.
- CS Med. Nobel Inst., Karolinska Inst., Stockholm, Swed.
- SO Exp. Cell Res. (1968), 50(1), 73-80 CODEN: ECREAL
- DΤ Journal

LA English

AB Quant. microspectrophotometric and microinterferometric analyses in combination with biochem. methods were used to examine the effects of 4-aminopyrazolo(3,4-d)pyrimidine (I) (5 .times. 10-6M) in combination with guanine (2 .times. 10-4M) on the synthesis of DNA, RNA, and protein in asynchronously growing Ehrlich ascites cells in culture. Exposure to such concns. of I + guanine resulted in a nonlethal inhibition of cell multiplication. Pulse labeling with thymidine-14C, uridine-14C, and leucine-1-14C in the presence of I + guanine revealed an exponential decline in the per cell rate of DNA synthesis, while the per cell rate of RNA synthesis, as adjudged by uridine-14C incorporation, was not significantly inhibited, and the per cell rate of protein synthesis was inhibited only .apprx.50%. Detn. of the cellular content of DNA, RNA, and protein by cytochem. population analyses revealed an accumulation of cells in G1 or early S-phase in I + quanine-treated cultures. These viable, but nondividing cells continued to incorporate uridine-14C and leucine-14C, but there was no net increase in either RNA or protein per cell; thus continued synthesis must be limited to RNA and protein which is constantly in the process of degradation and resynthesis. I + quanine may exert an inhibitory effect by interference with the synthesis and pool sizes of intracellular purine nucleotides.

IT 2380-63-4

RL: BIOL (Biological study)
 (nucleic acid and protein formation by carcinoma in response
 to quanine and)

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TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT. searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d ide can tot 1148

L148 ANSWER 1 OF 44 REGISTRY COPYRIGHT 2002 ACS
RN 119952-37-3 REGISTRY
CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4,6-diamino-1-.beta.-Dribofuranosyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H15 N7 O5

ME CIL HIS NA OS

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:173656

L148 ANSWER 2 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 119952-35-1 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4-amino-6-(methylthio)-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H16 N6 O5 S

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

Hit structure For ref 1-25

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:173656

L148 ANSWER 3 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 119952-34-0 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4,6-bis(methylthio)-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H17 N5 O5 S2

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:173656

L148 ANSWER 4 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **116019-28-4** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-amine, 6-methoxy-1-.beta.-D-ribofuranosyl-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H15 N5 O5

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:173656

REFERENCE 2: 109:93498

L148 ANSWER 5 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 107296-14-0 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-ethanamine, 4-amino-1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H18 N6 O3

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:214304

L148 ANSWER 6 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **96555-45-2** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 6-amino-4,5-dihydro-4-oxo-1-(2,3,5-tri-0-acetyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H20 N6 O9

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 103:37693

L148 ANSWER 7 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **96555-44-1** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 6-amino-4,5-dihydro-4-oxo-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 N6 O6

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 103:37693

L148 ANSWER 8 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **96555-43-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4,5-dihydro-6-(methylthio)-4-oxo-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C7 H7 N5 O2 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

$$\begin{array}{c|c} \text{MeS} & \overset{H}{N} & \overset{H}{N} \\ & \overset{N}{N} & \overset{N}{N} \\ & & \overset{C-NH_2}{N} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 103:37693

L148 ANSWER 9 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **96555-42-9** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4,5,6,7-tetrahydro-4-oxo-6-thioxo-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C6 H5 N5 O2 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

$$\begin{array}{c|c}
 & H & H \\
N & N \\
N & N \\
O & O \\
\end{array}$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 103:37693

L148 ANSWER 10 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **90914-52-6** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3,4(2H,5H)-dione, 1-.beta.-D-ribofuranosyl-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H12 N4 O6

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:97956

REFERENCE 2: 101:91391

L148 ANSWER 11 OF 44 REGISTRY COPYRIGHT 2002 ACS RN 90914-46-8 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4,5-dihydro-4-oxo-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H13 N5 O6

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 103:37693

REFERENCE 2: 101:91391

L148 ANSWER 12 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **90914-44-6** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3,4-diamine, 1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H14 N6 O4

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:91391

L148 ANSWER 13 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **90914-38-8** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 3-amino-1,5-dihydro-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H13 N5 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:165600

REFERENCE 2: 101:91391

L148 ANSWER 14 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 90914-32-2 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-3-(methylthio)-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 N4 O5 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER

(\*File contains numerically searchable property data)

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 101:91391

L148 ANSWER 15 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **85426-74-0** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-amino-1,5-dihydro-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-amino-1-.beta.-D-ribofuranosyl- (6CI) OTHER NAMES:

CN 7-Deaza-8-azaguanosine

FS STEREOSEARCH

MF C10 H13 N5 O5

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, MEDLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 9 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 9 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 126:43598

REFERENCE 2: 117:204404

REFERENCE 3: 113:172618

REFERENCE 4: 113:59760

REFERENCE 5: 112:77867

REFERENCE 6: 112:56530

REFERENCE 7: 106:207230

REFERENCE 8: 103:37693

REFERENCE 9: 98:179811

L148 ANSWER 16 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 78710-23-3 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-acetamide, 4,5-dihydro-6-(methylthio)-4-oxo-

1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H17 N5 O6 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 96:7014

REFERENCE 2: 95:98198

L148 ANSWER 17 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **78586-40-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-.beta.-D-ribofuranosyl- (6CI, 9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H12 N4 O4

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 6 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

6 REFERENCES IN FILE CAPLUS (1967 TO DATE) 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 123:52110

REFERENCE 2: 106:46285

REFERENCE 3: 98:100752

REFERENCE 4: 97:72700

REFERENCE 5: 96:45864

REFERENCE 6: 95:125862

L148 ANSWER 18 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **76690-46-5** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(methylthio)-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 N4 O5 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT (\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1967 TO DATE)

5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:56530

REFERENCE 2: 109:93507

REFERENCE 3: 96:7014

REFERENCE 4: 95:180745

REFERENCE 5: 94:103745

L148 ANSWER 19 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **76690-43-2** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,6-bis(methylthio)-1-(2,3,5-tri-O-acetyl-beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H22 N4 O7 S2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT (\*File contains numerically searchable property data)

## Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:93507

REFERENCE 2: 96:7014

REFERENCE 3: 94:103745

L148 ANSWER 20 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **74525-95-4** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(methylthio)-1-.beta.-D-

ribofuranosyl-, hydrazone (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H16 N6 O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1967 TO DATE)

5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:93498

REFERENCE 2: 96:7014

REFERENCE 3: 95:180745

REFERENCE 4: 94:103745

REFERENCE 5: 93:88460

L148 ANSWER 21 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 74525-93-2 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-amine, 6-(methylthio)-1-.beta.-D-

ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H15 N5 O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1967 TO DATE)

8 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:173656

REFERENCE 2: 109:93507

REFERENCE 3: 109:93498

REFERENCE 4: 98:179811

REFERENCE 5: 96:7014

REFERENCE 6: 95:180745

REFERENCE 7: 94:103745

REFERENCE 8: 93:88460

L148 ANSWER 22 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **74525-92-1** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,6-bis(methylthio)-1-.beta.-D-ribofuranosyl-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H16 N4 O4 S2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1967 TO DATE)

6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:56530

REFERENCE 2: 109:93498

REFERENCE 3: 96:7014

REFERENCE 4: 95:180745

REFERENCE 5: 94:103745

REFERENCE 6: 93:88460

L148 ANSWER 23 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **70421-30-6** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-4,6-diamine, 1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,6-diamino-1-.beta.-D-ribofuranosyl- (6CI)

FS STEREOSEARCH

MF C10 H14 N6 O4

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER (\*File contains numerically searchable property data)

## Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 2 REFERENCES IN FILE CA (1967 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 110:173656

REFERENCE 2: 91:15775

L148 ANSWER 24 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **70421-26-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-methoxy-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 N4 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:185380

REFERENCE 2: 95:125862

REFERENCE 3: 91:15775

L148 ANSWER 25 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **64372-77-6** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-.beta.-D-ribofuranosyl-, oxime (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H13 N5 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:125862

REFERENCE 2: 87:184865

L148 ANSWER 26 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **64372-76-5** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-.beta.-D-ribofuranosyl-, hydrazone (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H14 N6 O4

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER

(\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:72700

REFERENCE 2: 95:220260

REFERENCE 3: 95:125862

REFERENCE 4: 87:184865

L148 ANSWER 27 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **64372-72-1** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(2-propenylthio)-1-.beta.-D-ribofuranosyl-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H16 N4 O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1967 TO DATE) 5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:46285

REFERENCE 2: 98:100752

REFERENCE 3: 96:45864

REFERENCE 4: 95:125862

REFERENCE 5: 87:184865

L148 ANSWER 28 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **64372-69-6** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2,3,5-tri-0-acetyl-beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H18 N4 O8

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER (\*File contains numerically searchable property data)

Absolute stereochemistry.

5 REFERENCES IN FILE CA (1967 TO DATE)

5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:158770

REFERENCE 2: 97:163399

REFERENCE 3: 95:125862

REFERENCE 4: 95:62573

REFERENCE 5: 87:184865

L148 ANSWER 29 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **60355-67-1** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(methylthio)-1-.beta.-D-ribofuranosyl-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 N4 O4 S

LC STN Files: BEILSTEIN\*, CA, CANCERLIT, CAPLUS, MEDLINE, TOXCENTER (\*File contains numerically searchable property data)

# Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 18 REFERENCES IN FILE CA (1967 TO DATE)
- 18 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:52110

REFERENCE 2: 111:90073

REFERENCE 3: 110:165600

REFERENCE 4: 109:142123

REFERENCE 5: 106:46285

REFERENCE 6: 106:27490

REFERENCE 7: 102:197604

REFERENCE 8: 102:43384

REFERENCE 9: 98:100752

REFERENCE 10: 97:72700

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RN **60355-66-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(methylthio)-1-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H20 N4 O7 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:163399

REFERENCE 2: 96:7014

REFERENCE 3: 94:103745

REFERENCE 4: 85:108923

L148 ANSWER 31 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **55559-56-3** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-carboxamide, 4-amino-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Azasangivamycin

FS STEREOSEARCH

MF C11 H14 N6 O5

LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1967 TO DATE) 6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:125862

REFERENCE 2: 91:168263

REFERENCE 3: 91:117147

REFERENCE 4: 85:177891

REFERENCE 5: 84:159532

REFERENCE 6: 82:171339

L148 ANSWER 32 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **54524-71-9** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 8-Aza-6-mercapto-7-deazapurine riboside

FS STEREOSEARCH

MF C10 H12 N4 O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL (\*File contains numerically searchable property data)

Absolute stereochemistry.

19 REFERENCES IN FILE CA (1967 TO DATE)
19 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:52110

REFERENCE 2: 114:74707

REFERENCE 3: 110:165600

REFERENCE 4: 106:81433

REFERENCE 5: 106:46285

REFERENCE 6: 102:214677

REFERENCE 7: 102:105763

REFERENCE 8: 102:199

REFERENCE 9: 101:187866

REFERENCE 10: 99:133327

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RN **46153-15-5** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-ethanamine, 4-amino- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C7 H10 N6

CI COM

LC STN Files: CA, CAPLUS, CASREACT

$$\begin{array}{c|c} & H & N & N \\ N & N & N \\ N & NH_2 & CH_2 - CH_2 - NH_2 \end{array}$$

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:214304

L148 ANSWER 34 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN **24521-76-4** REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-mercapto- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidine-4,6(5H,7H)-dione, 6-thio-

CN 4-Hydroxy-6-mercaptopyrazolo[3,4-d]pyrimidine

CN B 103U

FS 3D CONCORD

DR 3323-96-4

MF C5 H4 N4 O S

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, EMBASE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

17 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

17 REFERENCES IN FILE CAPLUS (1967 TO DATE)

4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:180778

REFERENCE 2: 134:17496

REFERENCE 3: 133:357185

REFERENCE 4: 133:274164

REFERENCE 5: 133:36032

REFERENCE 6: 132:115157

REFERENCE 7: 129:182042

REFERENCE 8: 129:77920

REFERENCE 9: 126:137636

REFERENCE 10: 120:106914

L148 ANSWER 35 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 16220-07-8 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-.beta.-D-ribofuranosyl-(8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-Hydroxy[3,4-d]pyrazolopyrimidine riboside

CN Allopurinol ribonucleoside

CN Allopurinol riboside

CN Allopurinol-1-ribonucleoside

FS STEREOSEARCH

MF C10 H12 N4 O5

LC STN Files: AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMINFORMRX, DDFU, DRUGNL, DRUGU, DRUGUPDATES, EMBASE, IFICDB, IFIPAT, IFIUDB, MEDLINE, SPECINFO, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

97 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

97 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:25078

REFERENCE 2: 131:29442

REFERENCE 3: 128:189094

REFERENCE 4: 125:53806

REFERENCE 5: 124:25693

REFERENCE 6: 123:52110

REFERENCE 7: 122:230098

REFERENCE 8: 120:152877

REFERENCE 9: 120:107695

REFERENCE 10: 119:245177

L148 ANSWER 36 OF 44 REGISTRY COPYRIGHT 2002 ACS

RN 6288-89-7 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4,6-bis(methylthio)- (6CI, 8CI, 9CI) (CF INDEX NAME)

FS 3D CONCORD

MF C7 H8 N4 S2

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

21 REFERENCES IN FILE CA (1967 TO DATE)

21 REFERENCES IN FILE CAPLUS (1967 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 132:177005

REFERENCE 2: 125:58997

REFERENCE 3: 125:34025

REFERENCE 4: 124:117250

REFERENCE 5: 122:239865

REFERENCE 6: 120:217524

REFERENCE 7: 115:208428

REFERENCE 8: 114:102664

REFERENCE 9: 112:198289

REFERENCE 10: 112:56530

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RN **5418-10-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-(methylthio)- (6CI, 9CI) (CA INDEX NAME) OTHER NAMES:

CN 4-Methylthiopyrazolo[3,4-d]pyrimidine

FS 3D CONCORD

MF C6 H6 N4 S

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX, CHEMLIST, HODOC\*, TOXCENTER

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

21 REFERENCES IN FILE CA (1967 TO DATE)

21 REFERENCES IN FILE CAPLUS (1967 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:216978

REFERENCE 2: 134:208052

REFERENCE 3: 129:276241

REFERENCE 4: 127:109136

REFERENCE 5: 125:248292

REFERENCE 6: 124:176776

REFERENCE 7: 124:87669

REFERENCE 8: 122:239865

REFERENCE 9: 120:217524

REFERENCE 10: 118:7295

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RN 5334-26-9 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(methylthio)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-(methylthio)- (6CI, 8CI)

OTHER NAMES:

CN 6-(Methylthio)-1,7-dihydropyrazolo[3,4-d]pyrimidin-4-one

FS 3D CONCORD

MF C6 H6 N4 O S

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT,

IFIUDB, TOXCENTER

(\*File contains numerically searchable property data)

6 REFERENCES IN FILE CA (1967 TO DATE)

6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 134:17496

REFERENCE 2: 103:37693

REFERENCE 3: 95:180745

REFERENCE 4: 86:150384

REFERENCE 5: 79:78743

REFERENCE 6: 72:31827

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RN 3258-05-7 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-amine, 1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-amino-1-.beta.-D-ribofuranosyl- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Amino-1-(.beta.-d-ribofuranosyl)pyrazolo-[3,4-d]pyrimidine

CN 6-Azatubercidin

CN 7-Deaza-8-azaadenosine

FS STEREOSEARCH

DR 21247-86-9

MF C10 H13 N5 O4

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CHEMINFORMRX, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 37 REFERENCES IN FILE CA (1967 TO DATE)
- 37 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:63677

REFERENCE 2: 131:223117

REFERENCE 3: 126:16189

REFERENCE 4: 123:52110

REFERENCE 5: 119:91079

REFERENCE 6: 107:112526

REFERENCE 7: 107:19783

REFERENCE 8: 106:172780

REFERENCE 9: 106:46285

REFERENCE 10: 105:54102

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RN 2537-04-4 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-amino-1,5-dihydro- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-amino- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Hydroxy-6-aminopyrazolo[3,4-d]pyrimidine

CN 8-Aza-7-deazaguanine

CN HAPP

FS 3D CONCORD

MF C5 H5 N5 O

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, PHAR, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

18 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA'

18 REFERENCES IN FILE CAPLUS (1967 TO DATE)

11 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

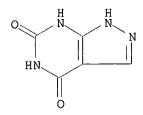
REFERENCE 1: 136:305109

REFERENCE 2: 135:15068

REFERENCE 3: 134:26053

REFERENCE 4: 131:296189

REFERENCE 5: 131:282379 REFERENCE 130:163642 6: REFERENCE 7: 129:185075 REFERENCE 8: 128:317694 REFERENCE 9: 118:7344 REFERENCE 10: 106:207230 L148 ANSWER 41 OF 44 REGISTRY COPYRIGHT 2002 ACS 2465-59-0 REGISTRY 1H-Pyrazolo[3,4-d]pyrimidine-4,6(5H,7H)-dione (7CI, 8CI, 9CI) (CA INDEX CN NAME) OTHER CA INDEX NAMES: 4H-Pyrazolo[3,4-d]pyrimidine-4,6(5H)-dione, 1,7-dihydro- (6CI) OTHER NAMES: CN 1H, 3H, 9H-Alloxanthine 1H-Pyrazolo[3,4-d]pyrimidin-4,6-diol CN 4,6-Dihydroxypyrazolo[3,4-d]pyrimidine CN CN Alloxanthine CN BW 55-5 Oxipurinol CN CN Oxoallopurinol CN Oxypurinol FS 3D CONCORD DR 16220-06-7, 22767-93-7, 4318-51-8 MF C5 H4 N4 O2 CI COM STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, LC BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DRUGNL, DRUGU, DRUGUPDATES, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, PHAR, PROMT, SPECINFO, TOXCENTER, USAN, USPATFULL, VETU (\*File contains numerically searchable property data) Other Sources: EINECS\*\*, WHO (\*\*Enter CHEMLIST File for up-to-date regulatory information)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 361 REFERENCES IN FILE CA (1967 TO DATE)
- 11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 361 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:15591

REFERENCE 2: 136:172182

REFERENCE 3: 136:163266

REFERENCE 4: 136:79508

REFERENCE 5: 136:107

REFERENCE 6: 135:251362

REFERENCE 7: 135:205240

REFERENCE 8: 135:148504

REFERENCE 9: 135:73328

REFERENCE 10: 135:15732

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RN **2380-63-4** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-amine (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-amino- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Amino-1H-pyrazolo[3,4-d]pyrimidine

CN 4-Aminopyrazolo[3,4-d]pyrimidine

CN 8-Aza-7-deazaadenine

FS 3D CONCORD

MF C5 H5 N5

CI COM

LC STN Files: BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, EMBASE, GMELIN\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, NIOSHTIC, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)
Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

193 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

193 REFERENCES IN FILE CAPLUS (1967 TO DATE)

49 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:396964

REFERENCE 2: 136:378311

REFERENCE 3: 136:377390

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REFERENCE
            4:
                136:305109
REFERENCE
                135:264486
            5:
REFERENCE
            6:
                135:180762
                135:101932
REFERENCE
            7:
                135:67903
REFERENCE
            8:
REFERENCE
            9:
                135:15068
REFERENCE 10:
                134:348925
L148 ANSWER 43 OF 44 REGISTRY COPYRIGHT 2002 ACS
     315-30-0 REGISTRY
     4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro- (7CI, 8CI, 9CI) (CA INDEX
CN
     NAME)
OTHER NAMES:
     1H-Pyrazolo[3,4-d]pyrimidin-4-ol
CN
     4-Hydroxy-1H-pyrazolo[3,4-d]pyrimidine
CN
     4-Hydroxypyrazolo[3,4-d]pyrimidine
CN
     Allopur
     Allopurinol
CN
     Allopurinol(I)
CN
CN
     Atisuril
CN
     Bloxanth
CN
     BW 56-158
CN
     Epidropal
CN
     Foligan
CN
     Gichtex
CN
     Gotax
CN
     HPP
CN
     Milurit
CN
     Uricemil
CN
     Uriprim
CN
     Urosin
CN
     Zyloprim
CN
     Zyloric
FS
     3D CONCORD
DR
     22767-92-6, 39464-14-7, 184856-42-6
MF
     C5 H4 N4 O
CI
     COM
                  ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS,
LC
     STN Files:
       BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN,
       CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGPAT, DRUGU, EMBASE,
       GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*,
       MSDS-OHS, NIOSHTIC, PHARMASEARCH, PROMT, RTECS*, SPECINFO, TOXCENTER,
       USAN, USPATFULL, VETU
         (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**, WHO
         (**Enter CHEMLIST File for up-to-date regulatory information)
```

1862 REFERENCES IN FILE CA (1967 TO DATE)

29 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1866 REFERENCES IN FILE CAPLUS (1967 TO DATE)

9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:24099

REFERENCE 2: 137:15717

REFERENCE 3: 137:15591

REFERENCE 4: 137:15456

REFERENCE 5: 137:3174

REFERENCE 6: 136:398181

REFERENCE 7: 136:397931

REFERENCE 8: 136:395267

REFERENCE 9: 136:395180

REFERENCE 10: 136:390902

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RN 271-80-7 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1H-Pyrazolyl(3,4-d)pyrimidine

CN 5H-Pyrazolo[3,4-d]pyrimidine

FS 3D CONCORD

DR 35760-86-2

MF C5 H4 N4

CI COM, RPS

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, MEDLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 45 REFERENCES IN FILE CA (1967 TO DATE)
- 27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 45 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:318825

REFERENCE 2: 136:179591

REFERENCE 3: 135:237547

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REFERENCE
           4: 135:15068
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               134:218320
           5:
               133:129894
REFERENCE
           6:
REFERENCE
               132:146163
           7:
               131:296189
REFERENCE
           8:
               130:206202
REFERENCE
           9:
               130:61060
REFERENCE 10:
=> d bib abs hitrn tot
L156 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
    1999:659532 HCAPLUS
DN
    131:296189
TI
    Oligonucleotides containing pyrazolo[3,4-d]pyrimidines for
    hybridization and mismatch discrimination
    Meyer, Rich B., Jr.; Afonina, Irina A.; Kutyavin, Igor V.
ΙN
PΑ
    Epoch Pharmaceuticals, Inc., USA
SO
    PCT Int. Appl., 51 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                     KIND DATE
                                         APPLICATION NO. DATE
                    ----
                                          -----
    WO 9951775
                           19991014
                                         WO 1999-US7492 19990405 <--
PΙ
                     A1
        W: AU, CA, JP
        RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
            PT, SE
                           20001003
                                          US 1998-54830
                                                           19980403
    US 6127121
                      Α
    CA 2327547
                           19991014
                                          CA 1999-2327547 19990405 <--
                      AA
    AU 9934724
                      A1
                           19991025
                                          AU 1999-34724
                                                          19990405 <--
    EP 1068358
                           20010117
                                          EP 1999-916394 19990405 <--
                      Α1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, FI
    JP 2002510507
                      T2
                           20020409
                                          JP 2000-542486
                                                           19990405 <--
PRAI US 1998-54830
                           19980403 <--
                      Α
    WO 1999-US7492
                      W
                           19990405
ΑB
    Oligonucleotides in which one or more purine residues are
    substituted by pyrazolo[3,4-d]pyrimidines exhibit improved hybridization
    properties. Oligonucleotides contg. pyrazolo[3,4-d]pyrimidine
    base analogs have higher melting temps. than unsubstituted
    oligonucleotides of identical sequence. Thus, in assays involving
    hybridization of an oligonucleotide probe to a target
    polynucleotide sequence, higher signals are obtained. In addn.,
    mismatch discrimination is enhanced when pyrazolo[3,4-d]pyrimidine-contg.
    oligonucleotides are used as hybridization probes, making them
    useful as probes and primers for hybridization, amplification and
    sequencing procedures, particularly those in which single- or multiple-
    nucleotide mismatch discrimination is required.
    271-80-7D, 1H-Pyrazolo[3,4-d]pyrimidine, derivs. 315-30-0
IT
    2380-63-4, 1H-Pyrazolo[3,4-d]pyrimidin-4-amine 2537-04-4
    RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
    BIOL (Biological study); OCCU (Occurrence)
        (oligonucleotides contg. pyrazolo[3,4-d]pyrimidines for
       hybridization and mismatch discrimination)
```

# RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L156 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
    1999:659404 HCAPLUS
DN
    131:282379
ΤI
    Hybridization and mismatch discrimination using oligonucleotides
    conjugated to minor groove binders
    Hedgpeth, Joel; Afonina, Irina A.; Kutyavin, Igor V.; Lukhtanov, Eugeny
IN
    A.; Belousov, Evgeniy S.; Meyer, Rich B., Jr.
    Epoch Pharmaceuticals, Inc., USA
PΑ
SO
    PCT Int. Appl., 95 pp.
    CODEN: PIXXD2
DT
    Patent
    English
T.A
FAN.CNT 3
    PATENT NO.
                     KIND DATE
                                         APPLICATION NO. DATE
                                         -----
    _____
                     ----
PI
    WO 9951621
                     A2
                           19991014
                                         WO 1999-US7487 19990405 <--
    WO 9951621
                     A3
                           20011108
        W: AU, CA, JP
        RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
            PT, SE
                           20011106
                                          US 1998-54832
                                                           19980403 <--
    US 6312894
                      В1
    CA 2329135
                           19991014
                                          CA 1999-2329135 19990405 <--
                      AA
    AU 9934721
                      A1
                           19991025
                                          AU 1999-34721
                                                           19990405 <--
                           20011017
                                          EP 1999-916391
                                                           19990405 <--
    EP 1144429
                      A2
           AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, FI
PRAI US 1998-54832
                           19980403
                      Α
                      A2
                           19950403
                                     <--
    US 1995-415370
                      W
                           19990405
    WO 1999-US7487
    Conjugates between a minor groove binding mol., such as the trimer of
AΒ
    1,2-dihydro-(3 H )-pyrrolo[3,2-e]indole-7-carboxylate (CDPI3), and an
    oligonucleotide form unusually stable hybrids with complementary
    target sequences, in which the tethered CDPI3 group resides in the minor
    groove of the duplex. These conjugates can be used as probes and primers.
    Due to their unusually high binding affinity, conjugates as short as
    8-mers can be used as amplification primers with high specificity and
    efficiency. Minor groove binder (MGB) conjugation also increases the
    discriminatory power of short oligonucleotides, providing
    enhanced detection of nucleotide sequence mismatches by short
    oligonucleotides. The MGB-conjugated probes and primers described
    herein facilitate various analytic and diagnostic procedures, such as
    amplification reactions, PCR, detection of single-nucleotide
    polymorphisms, gene hunting, differential display, fluorescence
    energy transfer, hydrolyzable probe assays and others; by allowing the use
    of shorter oligonucleotides, which have higher specificity and
    better discriminatory power.
ΙT
    2380-63-4, 4-Amino-1H-pyrazolo[3,4-d]pyrimidine 2465-59-0
    2537-04-4
    RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
    BIOL (Biological study); OCCU (Occurrence)
        (oligonucleotides conjugates contg.; hybridization and
       mismatch discrimination using oligonucleotides conjugated to
       minor groove binders)
L156 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
    1992:16348 HCAPLUS
ΑN
    116:16348
DN
ΤI
    A novel biotinylated adenylate analog derived from pyrazolo[3,4-
    d]pyrimidine for labeling DNA probes
```

Petrie, Charles R.; Adams, A. David; Stamm, Michael; Van Ness,

ΑU

```
Jeffery; Watanabe, Susan M.; Meyer, Rich B., Jr.
CS
     MicroProbe Corp., Bothell, WA, 98021, USA
     Bioconjugate Chem. (1991), 2(6), 441-6
SO
     CODEN: BCCHES; ISSN: 1043-1802
DT
     Journal
LA
     English
AΒ
     A novel dATP analog 3-[5-[(N-biotinyl-6-aminocaproyl)amino]pentyl]-1-(2-
     deoxy-.beta.-D-erythro-pentofuranosyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine
     5'-triphosphate, which is modified at the 3-position with a flexible
     linker arm bearing a terminal biotin moiety, was synthesized.
     nucleotide is readily incorporated into DNA probes by nick
     translation. These probes hybridize to complementary targets as well as
     probes labeled with bio-dUTP, as judged by slot blot. When
     incorporated into oligonucleotides, they do not cause the loss
     of hybridization efficiency that an N-6-substituted adenine
     nucleotide does when incorporated into the same sites in the
     oligonucleotide.
ΙT
     129357-76-2P
     RL: PREP (Preparation)
        (prepn. and deprotection and biotinylation of)
     129357-70-6P 129357-75-1P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and phosphorylation of)
IT
     137823-48-4P
     RL: PREP (Preparation)
        (prepn. of)
     137823-47-3P
ΙT
     RL: PREP (Preparation)
        (prepn. of, for labeling of DNA probes)
L156 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     1990:532717 HCAPLUS
     113:132717
DN
     Preparation of pyrazolo[3,4-d]pyrimidine derivatives as intermediates for
ΤI
     diagnostic oligonucleotides
IN
     Petrie, Charles R.; Meyer, Rich B.
     Microprobe Corp., USA
PA
     PCT Int. Appl., 41 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 8
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                             DATE
     WO 9003370
                      A1
                            19900405
                                           WO 1989-US4184
                                                             19890926 <--
PΙ
        W: JP
         RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE
                                           CA 1989-613651
                                                             19890927 <--
     CA 1338379
                      A1
                            19960611
     US 5824796
                                           US 1994-334490
                                                             19941104 <--
                            19981020
                       Α
PRAI US 1988-250474
                            19880928
                       Α
                                      <--
     US 1989-353857
                       В1
                            19890518
                                      <--
     US 1993-49807
                            19930420
                                      <--
                       В1
os
     MARPAT 113:132717
GI
```

AB The title compds. [I; R1 = H, sugar moiety optionally substituted at its 3' or 5' position with mono-, di-, or triphosphate or a reactive group suitable for nucleotide bond formation; provided that when R3 = H, R1 .noteq. H; R3 = H, W(X)nA; W, X = chem. linker arm; A = intercalator, electrophilic crosslinker, reporter group; R4, R6 = H, OH, SH, alkylthio, NH2, NH(CH2)tNH2; n = 0,1; t = 0-12] were prepd. by (1) reaction of 5-aminopyrazole-4-carbonitriles (II; R = cyano; R1, R3 = as above) with a dialkoxymethyl carboxylate followed by reaction with NH3 to give I (R4 = NH2), (2) reaction of II (R = CONH2; R1, R3 = as above) with a dialkoxymethyl carboxylate to give I (R4 = OH), or (3) reaction of II (R = cyano, CONH2; R1, R3 = as above) with an alkyl xanthate salt followed by an alkyl halide and oxidn. An oligonucleotide sequence contg. .gtoreq.1 of labeled I (R1 = sugar moiety as described above), particularly labeled with biotin, is used as DNA hybridization probe and as a kit for identifying target DNA sequence comprising the above labeled oligonucleotide complementary to the target DNA, a denaturation reagent, and a hybridization reaction mixt. (no data). Thus, 5-amino-1-(2-deoxy-3,5-di-O-toluoyl-.beta.-D-erythropentofuranosyl)-3-[(5tritylamino)pentyl]pyrazole-4-carbonitrile was heated 5 h at 80-90.degree. with AcOCH2(OEt)2 and the intermediate syrup was treated 2 days at room temp. with methanolic NH3 to give 77% I [R1 = Q, R2 = R6 = H, R3 = (CH2)5NHCPh3, R4 = NH2]. This was phosphorylated by reaction with POCl3 in (MeO) 3PO followed by hydrolysis with 0.1 M NH4HCO3 to give I [R1 = Q,R2 = (HO)2P(O), R3 = (CH2)5NHCPh3, R4 = NH2, R6 = H] which was hydrogenolyzed over Pd(OH)2/C in cyclohexadiene and then acylated with N-hydroxysuccinimidyl 6-biotinamidocaproate in DMF contg. Et3N to give I [R1 = Q, R2 = (HO)2P(O), R3 = 5-[(6-biotinamido)hexamido]pentyl, R4 = NH2,R6 = H].

IT 129357-75-1P 129357-76-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of biotin-labeled deoxyribofuranosylpyrazolopyrimidine nucleotide)

IT 129357-70-6P 129357-71-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for oligonucleotide hybridization
 probes)

=> d ide can tot

L158 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 137823-48-4 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-pentanamine, 4-amino-N-(triphenylmethyl)-(9CI) (CA INDEX NAME)

MF C29 H30 N6

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} N & H \\ N & N \\ N & \\ NH_2 & \\ \end{array}$$
 (CH<sub>2</sub>) 5-NH-CPh<sub>3</sub>

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 116:16348

L158 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 129357-76-2 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-pentanamine, 4-amino-1-(2-deoxy-5-0-phosphono-.beta.-D-erythro-pentofuranosyl)-N-(triphenylmethyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C34 H39 N6 O6 P

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1967 TO DATE)

5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:330802

REFERENCE 2: 126:153646

REFERENCE 3: 119:221156

REFERENCE 4: 116:16348

REFERENCE 5: 113:132717

L158 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2002 ACS RN 129357-75-1 REGISTRY

#### owens - 09 / 693213

CN 1H-Pyrazolo[3,4-d]pyrimidine-3-pentanamine, 4-amino-1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-N-(triphenylmethyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C34 H38 N6 O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

# Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1967 TO DATE) 5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:330802

REFERENCE 2: 126:153646

REFERENCE 3: 119:221156

REFERENCE 4: 116:16348

REFERENCE 5: 113:132717

L158 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 2537-04-4 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-amino-1,5-dihydro- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-amino- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Hydroxy-6-aminopyrazolo[3,4-d]pyrimidine

CN 8-Aza-7-deazaguanine

CN HAPP

FS 3D CONCORD

MF C5 H5 N5 O

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, PHAR, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

18 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

18 REFERENCES IN FILE CAPLUS (1967 TO DATE)

11 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:305109

REFERENCE 2: 135:15068

REFERENCE 3: 134:26053

REFERENCE 4: 131:296189

REFERENCE 5: 131:282379

REFERENCE 6: 130:163642

REFERENCE 7: 129:185075

REFERENCE 8: 128:317694

REFERENCE 9: 118:7344

REFERENCE 10: 106:207230

L158 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN **2465-59-0** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine-4,6(5H,7H)-dione (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 4H-Pyrazolo[3,4-d]pyrimidine-4,6(5H)-dione, 1,7-dihydro- (6CI)

OTHER NAMES:

CN 1H, 3H, 9H-Alloxanthine

CN 1H-Pyrazolo[3,4-d]pyrimidin-4,6-diol

CN 4,6-Dihydroxypyrazolo[3,4-d]pyrimidine

CN Alloxanthine

CN BW 55-5

CN Oxipurinol

CN Oxoallopurinol

CN Oxypurinol

FS 3D CONCORD

DR 16220-06-7, 22767-93-7, 4318-51-8

MF C5 H4 N4 O2

CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*,
BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT,
CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DRUGNL, DRUGU,
DRUGUPDATES, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, PHAR, PROMT,
SPECINFO, TOXCENTER, USAN, USPATFULL, VETU

(\*File contains numerically searchable property data)
Other Sources: EINECS\*\*, WHO
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

361 REFERENCES IN FILE CA (1967 TO DATE)

11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

361 REFERENCES IN FILE CAPLUS (1967 TO DATE) 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:15591

REFERENCE 2: 136:172182

REFERENCE 3: 136:163266

REFERENCE 4: 136:79508

REFERENCE 5: 136:107

REFERENCE 6: 135:251362

REFERENCE 7: 135:205240

REFERENCE 8: 135:148504

REFERENCE 9: 135:73328

REFERENCE 10: 135:15732

L158 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 2380-63-4 REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-amine (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-amino- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Amino-1H-pyrazolo[3,4-d]pyrimidine

CN 4-Aminopyrazolo[3,4-d]pyrimidine

CN 8-Aza-7-deazaadenine

FS 3D CONCORD

MF C5 H5 N5

CI COM

LC STN Files: BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, EMBASE, GMELIN\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, NIOSHTIC, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)
Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

193 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

193 REFERENCES IN FILE CAPLUS (1967 TO DATE)

49 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:396964

REFERENCE 2: 136:378311

REFERENCE 3: 136:377390

REFERENCE 4: 136:305109

REFERENCE 5: 135:264486

REFERENCE 6: 135:180762

REFERENCE 7: 135:101932

REFERENCE 8: 135:67903

REFERENCE 9: 135:15068

REFERENCE 10: 134:348925

L158 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 315-30-0 REGISTRY

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro- (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol

CN 4-Hydroxy-1H-pyrazolo[3,4-d]pyrimidine

CN 4-Hydroxypyrazolo[3,4-d]pyrimidine

CN Allopur

CN Allopurinol

CN Allopurinol(I)

CN Atisuril

CN Bloxanth

CN BW 56-158

CN Epidropal

CN Foligan

CN Gichtex

CN Gotax

CN HPP

CN Milurit

CN Uricemil

CN Uriprim

CN Urosin CN Zyloprim CN Zyloric FS 3D CONCORD 22767-92-6, 39464-14-7, 184856-42-6 DR MF C5 H4 N4 O CI COM ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, LC STN Files: BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGPAT, DRUGU, EMBASE, GMELIN\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC, PHARMASEARCH, PROMT, RTECS\*, SPECINFO, TOXCENTER, USAN, USPATFULL, VETU (\*File contains numerically searchable property data) DSL\*\*, EINECS\*\*, TSCA\*\*, WHO (\*\*Enter CHEMLIST File for up-to-date regulatory information)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1862 REFERENCES IN FILE CA (1967 TO DATE)
29 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1866 REFERENCES IN FILE CAPLUS (1967 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:24099

REFERENCE 2: 137:15717

REFERENCE 3: 137:15591

REFERENCE 4: 137:15456

REFERENCE 5: 137:3174

REFERENCE 6: 136:398181

REFERENCE 7: 136:397931

REFERENCE 8: 136:395267

REFERENCE 9: 136:395180

REFERENCE 10: 136:390902

L158 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN **271-80-7** REGISTRY

CN 1H-Pyrazolo[3,4-d]pyrimidine (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1H-Pyrazolyl(3,4-d)pyrimidine

CN 5H-Pyrazolo[3,4-d]pyrimidine

FS 3D CONCORD

DR 35760-86-2

MF C5 H4 N4

CI COM, RPS

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, MEDLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

45 REFERENCES IN FILE CA (1967 TO DATE)

27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

45 REFERENCES IN FILE CAPLUS (1967 TO DATE)

4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:318825

REFERENCE 2: 136:179591

REFERENCE 3: 135:237547

REFERENCE 4: 135:15068

REFERENCE 5: 134:218320

REFERENCE 6: 133:129894

REFERENCE 7: 132:146163

REFERENCE 8: 131:296189

REFERENCE 9: 130:206202

REFERENCE 10: 130:61060

## => fil hcaplus

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FILE COVERS 1907 - 9 Jul 2002 VOL 137 ISS 2 FILE LAST UPDATED: 8 Jul 2002 (20020708/ED) This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

```
=> d all tot 1184
```

```
L184 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2002 ACS
```

2000:754456 HCAPLUS ΑN

DN 133:306344

ΤI Targeted mutagenesis in living cells using modified oligonucleotides

Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall, ΤN Alexander A.

PΑ Epoch Pharmaceuticals, Inc., USA

U.S., 19 pp., Cont.-in-part of U.S. 5,849,482. SO CODEN: USXXAM

DT Patent

English LA

IC ICM C12Q001-68 ICS C07H021-04

NCL 435375000

3-2 (Biochemical Genetics) CC

Section cross-reference(s): 10, 11, 12,

FAN. CNT 8								
	PATENT NO.		KIND	DATE		AF J 2 W		
ΡΙ		6136601	A	20001024		T T		
PRAI		5849482 1991-748138	A B1	19981215 19910821		בבט טיידיים פרבר־US		\ <
11011		1994-178733	B2	19940107				
,	US	1995-485611	A2	19950607				
	~ ~	1988-250474	B2	19880928	<			
	US	1989-353857	B1	19890518		•		
	US	1993-11482	B2	19930126				
	US	1993-49807	B1	19930420				
	US	1994-226949	A2	19940627				
	US	1994-334490	Α	19941104			*	

This pour

A method for introducing a site-specific mutation into a target AΒ polynucleotide sequence is presented. The method involves the use of an oligonucleotide capable of binding to the target sequence, either by triplex formation (mediated by Hoogsteen, reverse Hoogsteen or equiv. base pairing) or by Watson/Crick base pairing (in the presence of a recombinase enzyme). The oligonucleotide of the invention is modified by the covalent attachment of one or more electrophilic groups. When a modified oligonucleotide is bound to its target sequence, the electrophilic group is able to interact with a nearby nucleotide in the target sequence, causing a modification to the nucleotide that results in a change in nucleotide sequence. Compns. used in the practice of the method are also disclosed.

ST target mutagenesis living cell modification oligonucleotide

ΙT Animal cell line

(COS; targeted mutagenesis in living cells using modified oligonucleotides)

Quaternary structure ΙT

(DNA triplex; targeted mutagenesis in living cells using modified oligonucleotides)

ΙT Enzymes, biological studies RL: BSU (Biological study, unclassified); CAT (Catalyst use); BIOL (Biological study); USES (Uses)

```
(DNA-recombining, oligonucleotide with; targeted mutagenesis
        in living cells using modified oligonucleotides)
ΙT
    Escherichia coli
        (MBM7070, transformation by electroporation; targeted mutagenesis in
        living cells using modified oligonucleotides)
IT
     Chromosome
        (animal; targeted mutagenesis in living cells using modified
       oligonucleotides)
ΙT
    Crosslinking
        (between oligonucleotide and plasmid; targeted mutagenesis in
        living cells using modified oligonucleotides)
ΙT
     Pathogen
        (genome of, mutagenesis of target sequence; targeted mutagenesis in
        living cells using modified oligonucleotides)
IT
        (pSP189; targeted mutagenesis in living cells using modified
        oligonucleotides)
IT
    Chromosome
        (plant, target sequence in; targeted mutagenesis in living cells using
       modified oligonucleotides)
IT
    Mutagenesis
        (site-directed; targeted mutagenesis in living cells using modified
        oligonucleotides)
TΤ
    Gene, animal
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP
     (Properties); BIOL (Biological study); OCCU (Occurrence)
        (supF; targeted mutagenesis in living cells using modified
        oligonucleotides)
TΤ
    Animal tissue culture
     Electroporation
     Transformation, genetic
        (targeted mutagenesis in living cells using modified
        oligonucleotides)
IΤ
    Oligonucleotides
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); BIOL (Biological study)
        (targeted mutagenesis in living cells using modified
        oligonucleotides)
IT
    Genome
        (viral, of pathogen; targeted mutagenesis in living cells using
        modified oligonucleotides)
TΤ
    Mutagens
        (with electrophilic group or alkylating agent; targeted mutagenesis in
        living cells using modified oligonucleotides)
     55-86-7, Nitrogen mustard
IT
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (bifunctional, alkylating group; targeted mutagenesis in living cells
        using modified oligonucleotides)
                                             237059-49-3D,
     171258-27-8D, oligonucleotides contg.
ΤТ
     oligonucleotides contg.
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (targeted mutagenesis in living cells using modified
        oligonucleotides)
     6872-73-7, Coralyne
IT
     RL: ARU (Analytical role, unclassified); ANST (Analytical study)
        (triplex stabilizer; targeted mutagenesis in living cells using
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TT
     US6136601 SEQID: 6 unclaimed DNA
                                       302479-28-3, 3: PN: US6136601 SEQID: 7
     unclaimed DNA
                     302479-29-4, 4: PN: US6136601 SEQID: 8 unclaimed DNA
     302479-30-7, 5: PN: US6136601 SEQID: 9 unclaimed DNA
                                                             302479-31-8, 6: PN:
                                        302479-32-9, 8: PN: US6136601 SEQID: 3
     US6136601 SEQID: 1 unclaimed DNA
                     302479-33-0, 9: PN: US6136601 SEQID: 4 unclaimed DNA
     unclaimed DNA
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RL: PRP (Properties)

(unclaimed nucleotide sequence; targeted mutagenesis in living cells using modified oligonucleotides) IT 302479-34-1 RL: PRP (Properties) (unclaimed sequence; targeted mutagenesis in living cells using modified oligonucleotides) THERE ARE 133 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 133 RE (1) Agrawal; Nucleic Acids Res 1990, V18(18), P5419 HCAPLUS (2) Anon; EP 021293 1981 HCAPLUS (3) Anon; DE 3310337 1984 HCAPLUS (4) Anon; WO 8403285 1984 HCAPLUS (5) Anon; WO 8502628 1985 HCAPLUS (6) Anon; WO 8503075 1985 HCAPLUS (7) Anon; EP 198207 1986 HCAPLUS (8) Anon; EP 214908 1986 HCAPLUS (9) Anon; JP 61109797 1986 HCAPLUS (10) Anon; WO 8602929 1986 HCAPLUS (11) Anon; WO 8604816 1986 HCAPLUS (12) Anon; WO 9641008 1986 HCAPLUS (13) Anon; EP 227459 1987 HCAPLUS (14) Anon; EP 242264 1987 HCAPLUS (15) Anon; WO 8707611 1987 HCAPLUS (16) Anon; EP 259186 1988 HCAPLUS (17) Anon; EP 266099 1988 HCAPLUS (18) Anon; EP 267996 1988 HCAPLUS (19) Anon; WO 8810264 1988 HCAPLUS (20) Anon; EP 375406 1989 HCAPLUS (21) Anon; EP 375408 1990 HCAPLUS (22) Anon; WO 9003370 1990 HCAPLUS (23) Anon; WO 9014353 1990 HCAPLUS (24) Anon; WO 9015884 1990 HCAPLUS (25) Anon; WO 9118997 1991 HCAPLUS (26) Anon; WO 9220698 1992 HCAPLUS (27) Anon; WO 9303736 1993 HCAPLUS (28) Anon; WO 9417092 1994 HCAPLUS (29) Anon; WO 9501364 1995 HCAPLUS (30) Anon; WO 9639195 1996 HCAPLUS (31) Anon; WO 9640271 1996 HCAPLUS (32) Anon; WO 9640711 1996 HCAPLUS (33) Anon; WO 9640898 1996 HCAPLUS (34) Arrand; Nucleic Acid Hybridisation 1985, P17 (35) Averbeck, D; Mutation Res 1985, V151, P217 HCAPLUS (36) Baker, B; Design of Active-Site Directed Irreversible Enzyme Inhibitors (37) Bergstrom, D; J Amer Chem Soc 1978, V100(26), P8106 HCAPLUS (38) Bigge, C; J Amer Chem Soc 1980, V102(6), P2033 HCAPLUS (39) Blake; Biochemistry 1985, V24, P6139 HCAPLUS (40) Bolli, M; Nucleic Acids Res 1996, V24, P4660 HCAPLUS (41) Brown, T; Oligonucleotides and Analogues: A practical approach 1991, P1 (42) Busso, M; AIDS Research and Human Retroviruses 1988, V4(6), P449 HCAPLUS (43) Calabresi, P; The Pharmacological Basis of Therapeutics, 8th ed 1990, P1202 (44) Camerini-Otero, R; Method of Forming three Stranded DNA, National Institutes of Health 1990 (45) Chatterjee, M; J Am Chem Soc 1990, V112, P6397 HCAPLUS (46) Cheng, S; J Biol Chem 1988, V263(15), P110 (47) Cooney, M; Scienie V241, P456 HCAPLUS (48) Crooke; Antisense Research and Development 1994, V4, P145 MEDLINE (49) Dale, R; Biochemistry 1975, V14(11), P2447 HCAPLUS (50) Dale, R; Proc Natl Acad Sci USA 1973, V70(8), P2238 HCAPLUS

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ΑN
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    Targeted mutagenesis in living cells using modified
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    oligonucleotides
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    Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall,
    Alexander A.
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    Epoch Pharmaceuticals, Inc., USA
    U.S., 20 pp.
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    ICM C12N015-00
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    3-2 (Biochemical Genetics)
    Section cross-reference(s): 13
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                     B2
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                    A2
    US 1994-226949
                           19940627
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AB A method for introducing a site-specific mutation into a target polynucleotide sequence is presented. The method involves the use of an oligonucleotide capable of binding to the target sequence, either by triplex formation (mediated by Hoogsteen, reverse Hoogsteen or equiv. base pairing) or by Watson/Crick base pairing (in the presence of a recombinase enzyme). The oligonucleotide of the invention is modified by the covalent attachment of one or more electrophilic groups. When a modified oligonucleotide is bound to its target sequence, the electrophilic group is able to interact with a nearby

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(9) Anon; WO 86/02929 1986 HCAPLUS

nucleotide in the target sequence, causing a modification to the nucleotide that results in a change in nucleotide sequence. Compns. used in the practice of the method are disclosed. disclosed are arm-leaving group structure having the formula -A-L such as (CH2)qY(CH2)mL, (CH2)qNHCO(CH2)m(X)n'N(R1)(CH2)pL, or (CH2)q'O(CH2)q''NHCO(CH2)m(X)n'N(R1)(CH2)pL (q=0-8, q'=1-7; Y=NH2, OH, SH,COOH, C.ident.CH; X= (Cl, Br, lower alkyl, lower alkoxy-substituted) Ph; n'=0, 1; p=1-6; R1=H, lower alkyl, or (CH2)pL; L=C1, Br, I, SO2R2, S+R3; R3,R4=C1-6 alkyl, aryl, heteroaryl, or R3 and R4 form a C1-6-alkylene bridge). target mutagenesis living cell modification oligonucleotide Quaternary structure (DNA triplex; targeted mutagenesis in living cells using modified oligonucleotides) Enzymes, biological studies RL: BSU (Biological study, unclassified); CAT (Catalyst use); BIOL (Biological study); USES (Uses) (DNA-recombining, oligonucleotide with; targeted mutagenesis in living cells using modified oligonucleotides) Plasmids (pSP189; targeted mutagenesis in living cells using modified oligonucleotides) Chromosome (plant, animal; target sequence; targeted mutagenesis in living cells using modified oligonucleotides) Mutagenesis (site-directed; targeted mutagenesis in living cells using modified oligonucleotides) Gene, animal RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (supF; targeted mutagenesis in living cells using modified oligonucleotides) Animal tissue culture (targeted mutagenesis in living cells using modified oligonucleotides) Genome (viral, of pathogen; target sequence; targeted mutagenesis in living cells using modified oligonucleotides) 55-86-7, Nitrogen mustard RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (bifunctional, alkylating group; targeted mutagenesis in living cells using modified oligonucleotides) 171258-27-8D, oligonucleotides contg. 237059-49-3D, oligonucleotides contg. RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (targeted mutagenesis in living cells using modified oligonucleotides) 6872-73-7, Coralyne RL: ARU (Analytical role, unclassified); ANST (Analytical study) (triplex stabilizer; targeted mutagenesis in living cells using modified oligonucleotides) THERE ARE 155 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 155 (1) Agrawal; Nucleic Acids Res 1990, V18(18), P5419 HCAPLUS (2) Anon; EP 021293 1981 HCAPLUS (3) Anon; DE 3310337 1984 HCAPLUS (4) Anon; WO 84/03285 1984 HCAPLUS (5) Anon; WO 85/02628 1985 HCAPLUS (6) Anon; WO 85/03075 1985 HCAPLUS (7) Anon; EP 198207 1986 HCAPLUS (8) Anon; JP 61-109797 1986 HCAPLUS

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L184 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN
    1997:148844 HCAPLUS
    126:153646
DN
ΤI
    Oligonucleotide derivs. preparation for target nucleic
     acid alkylation and crosslinking, gene mapping, and gene therapy
    Meyer, Rich B., Jr.; Gamper, Howard B.; Kutyavin, Igor V.; Gall,
IN
    Alexander A.; Petrie, Charles R.; Tabone, John C.;
    Hurst, Gerald D.
    Microprobe Corporation, USA
PA
     PCT Int. Appl., 91 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LA
    English
IC
     ICM C07H021-00
CC
     3-1 (Biochemical Genetics)
     Section cross-reference(s): 1, 33
FAN.CNT 8
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             MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT,
             UA, UG
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
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                      Α1
                            19980520
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             IE, FI
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                                                            19960607
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     US 1988-250474
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     US 1989-353857
                       В1
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AΒ

ST

IT

TΤ

TT

TT

TΤ

IT

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US 1991-748138
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US 1993-11482
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US 1993-49807
                  В1
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US 1994-178733
                 B2
                      19940107
US 1994-226949
                 A2
                       19940627
US 1994-334490
                       19941104
                  Α
WO 1996-US9551
                  W
                       19960607
Oligonucleotide derivs. (ODNs) include a sequence that is
complementary to a target sequence in single-stranded RNA, or single- or
double-stranded DNA, and an alkylating function which after hybridization
alkylates the target sequence. ODNs adapted for alkylating
single-stranded RNA, such as mRNA, are complementary to the target
sequence in the Watson Crick sense. ODNs adapted for alkylating
double-stranded DNA have at least two alkylating functions and are
complementary to the target sequence in the Hoogsteen or reverse Hoogsteen
sense. With these ODNs both strands of the target sequence are alkylated.
A third class of ODNs have at least approx. 26 nucleotide units
in a continuous sequence which are complementary to the target sequence of
double-stranded DNA, and the alkylating function is covalently attached to
a nucleotide unit in the continuous sequence. Alkylation or
crosslinking with this class of ODNs occurs in the presence of a
recombinase enzyme.
oligonucleotide deriv alkylating crosslinking agent
gene; mapping gene oligonucleotide deriv alkylating
crosslinking; therapy gene oligonucleotide deriv-
alkylating crosslinking
Enzymes, uses
RL: CAT (Catalyst use); USES (Uses)
   (DNA-recombining, in recombinase presence; oligonucleotide
   derivs. prepn. for target nucleic acid alkylation and
   crosslinking, gene mapping, and gene therapy)
Oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); CAT
(Catalyst use); SPN (Synthetic preparation); THU (Therapeutic use); ANST
(Analytical study); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (derivs.; oligonucleotide derivs. prepn. for target
   nucleic acid alkylation and crosslinking, gene
   mapping, and gene therapy)
DNA
RL: ANT (Analyte); BUU (Biological use, unclassified); THU (Therapeutic
use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
   (double-stranded; oligonucleotide derivs. prepn. for target
   nucleic acid alkylation and crosslinking, gene
   mapping, and gene therapy)
Oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); CAT
(Catalyst use); SPN (Synthetic preparation); THU (Therapeutic use); ANST
(Analytical study); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (haloacylamidoalkyl derivs.; oligonucleotide derivs. prepn.
   for target nucleic acid alkylation and crosslinking
   , gene mapping, and gene therapy)
Alkylating agents, biological
  Crosslinking agents
Gene therapy
  Genetic mapping
   (oligonucleotide derivs. prepn. for target nucleic
   acid alkylation and crosslinking, gene mapping, and gene
mRNA
```

RL: ANT (Analyte); BUU (Biological use, unclassified); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)

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(oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
IT
     Probes (nucleic acid)
     RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); CAT
     (Catalyst use); SPN (Synthetic preparation); THU (Therapeutic use); ANST
     (Analytical study); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
IT
    Gene
        (regulation, inhibition; oligonucleotide derivs. prepn. for
        target nucleic acid alkylation and crosslinking,
        gene mapping, and gene therapy)
IT
     DNA
    RL: ANT (Analyte); BUU (Biological use, unclassified); THU (Therapeutic
     use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
        (single-stranded; oligonucleotide derivs. prepn. for target
       nucleic acid alkylation and crosslinking, gene
        mapping, and gene therapy)
     123265-52-1D, oligonucleotide derivs.
     186696-57-1D, oligonucleotide derivs.
     186696-58-2D, oligonucleotide derivs.
     186696-59-3D, oligonucleotide derivs.
     RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); CAT
     (Catalyst use); THU (Therapeutic use); ANST (Analytical study); BIOL
     (Biological study); USES (Uses)
        (oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
IT
     161601-18-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with iododeoxyuridine; oligonucleotide
        derivs. prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
     5612-13-5P, 6-(Tritylamino)caproic acid
ΤТ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with malononitrile or cyanoacetamide;
        oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
IΤ
     161601-17-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with oligonucleotide salts;
        oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
     129357-70-6P
                    129357-73-9P
                                   129357-74-0P
                                                  129357-75-1P
                                                                  129357-76-2P
TΤ
                    142685-25-4P 161601-19-0P
     137823-46-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction; oligonucleotide derivs. prepn. for
        target nucleic acid alkylation and crosslinking,
        gene mapping, and gene therapy)
     129357-72-8P
TΤ
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction; oligonucleotide derivs. prepn. for
        target nucleic acid alkylation and crosslinking,
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gene mapping, and gene therapy)
ΙT
     134140-85-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and redn.; oligonucleotide derivs. prepn. for target
        nucleic acid alkylation and crosslinking, gene
        mapping, and gene therapy)
     134141-36-9P
                    137823-47-3P 161601-20-3P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn.; oligonucleotide derivs. prepn. for target
        nucleic acid alkylation and crosslinking, gene
        mapping, and gene therapy)
IT
     76-83-5, Trityl chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with aminocaproic acid; oligonucleotide derivs.
        prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy),
IT
    3601-89-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with carbonitrile deriv.; oligonucleotide derivs.
        prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
TΤ
     14396-90-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with iododeoxyuridine; oligonucleotide derivs.
        prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
IT
     72040-63-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with nucleotide deriv.; oligonucleotide
        derivs. prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
ΙT
     54-42-2
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with phthalimido-butyne or (trifluoroacetamidoethoxy)propyne;
        oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
     14036-06-7, Diethoxymethyl acetate
TT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with pyrazole carbonitrile deriv.; oligonucleotide
        derivs. prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
TΤ
     407-25-0, Trifluoroacetic anhydride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with tetrafluorophenol; oligonucleotide derivs.
        prepn. for target nucleic acid alkylation and
        crosslinking, gene mapping, and gene therapy)
IT
     305-03-3DP, Chlorambucil, oligonucleotide derivs.
     RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); CAT
     (Catalyst use); SPN (Synthetic preparation); THU (Therapeutic use); ANST
     (Analytical study); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (reaction with tetrafluorophenyl trifluoroacetate;
        oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
     305-03-3, Chlorambucil
TΤ
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with tetrafluorophenyl trifluoroacetate;
        oligonucleotide derivs. prepn. for target nucleic
        acid alkylation and crosslinking, gene mapping, and gene
        therapy)
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IT
     769-39-1, 2,3,5,6-Tetrafluorophenol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with trifluoroacetic acid; oligonucleotide derivs.
       prepn. for target nucleic acid alkylation and
       crosslinking, gene mapping, and gene therapy)
ΙT
     109-77-3, Malononitrile
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with tritylamino caproic acid; oligonucleotide
       derivs. prepn. for target nucleic acid alkylation and
       crosslinking, gene mapping, and gene therapy)
IT
     60-32-2, 6-Aminocaproic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (tritylation; oligonucleotide derivs. prepn. for target
       nucleic acid alkylation and crosslinking, gene
       mapping, and gene therapy)
L184 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN
    1991:409259 HCAPLUS
DN
    115:9259
TΙ
    Preparation of crosslinking oligonucleotides as
    nucleic acid hybridization probes
    Petrie, Charles R.; Meyer, Richard B.; Tabone,
IN
     John C.; Hurst, Gerald D.
PA
    Microprobe Corp., USA
SO
    PCT Int. Appl., 42 pp.
    CODEN: PIXXD2
DT
     Patent
    English
LA
IC
    ICM C07H021-00
     ICS C12Q001-68; C12Q001-70; G01N033-53
CC
     33-9 (Carbohydrates)
     Section cross-reference(s): 9
FAN.CNT 8
    PATENT NO.
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    WO 9014353
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                            19901129
                                          WO 1990-US2740
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     EP 472648
                     A1 19920304
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                                           JP 1990-508242
     JP 04507402
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                                                            19900515
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     US 5824796
                                                          19941104 <--
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PRAI US .1989-353857
                            19890518
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    US 1988-250474
                      B2
                            19880928
                                     <--
    WO 1990-US2740
                      W
                            19900515
    US 1993-49807
                      В1
                            19930420
OS
    MARPAT 115:9259
AB
    R1-B-(CH2)q-Yr-(CH2)m-A1 [R1 = H, sugar (analog) moiety optionally contg.
    Q1, Q2, Q3, P, etc.; Q1 = OH, OP(O)(OH)2, OP(O)(OH)OP(O)(OH)2; Q2 = O, \tilde{S};
     Q3 = CH2R2, SR2, OR2, NR2R3; R2, R3 = H, alkyl; B = nucleic acid
    base or an analog thereof; Y = functional linking group; m, q = 0, 1-8
     integer; r = 0, 1; A1 = leaving group], useful as nucleic acid
     hybridization probes and therefore useful for diagnosis of diseases, were
    prepd. Reaction of 5-iodo-2'-deoxyuridine in DMF with
     4-phthalimido-1-butyne in the presence of (Ph3P)4Pd and Et3N at 60.degree.
     for 3 h gave 5-(4-phthalimido-1-butyn-1-yl)-2'-deoxyuridine, whose
     hydrogenation over Raney Ni gave 5-(4-phthalimidobutyl)-2'-deoxyuridine.
     5-[3-(Trifluoroacetamido)propyl]-2'-deoxyuridine was prepd. similarly and
     converted according to known methods into 5'-O-(dimethoxytrity1)-2'-
     deoxyuridine-3'-(N,N-diisopropyl)phosphoramidite cyanoethyl ester, which
     was used in the automated synthesis of 3'-CT TCC U1TG TAG CTG-5' [I; U1 =
     5-(3-aminopropyl)-2'-deoxyuridine residue]. This was reacted with
     N-(iodoactoxy)succinimide to give II [U1 = 5-(3-iodoacetamidopropyl)-2'-
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uridine residue], whose crosslinking to a 30-mer
     oligonucleotide derived from human papillomavirus (HPV) was
     evaluated.
ST
     crosslinking oligonucleotide prepn; nucleic
     acid hybridization probe
IT
     Nucleic acid hybridization
        (probes, crosslinking oligonucleotides for)
ΙT
     Diagnosis
        (agents, nucleic acid hybridization probes in,
        crosslinking oligonucleotides as)
IT
     Nucleotides, polymers
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (oligo-, crosslinking, prepn. of, as probes for
        nucleic acid hybridization)
ΙT
     14396-90-8
     RL: RCT (Reactant)
        (alkylation by, of iododeoxyuridine)
     54-42-2, 5-Iodo-2'-deoxyuridine
IT
     RL: RCT (Reactant)
        (alkynylation of)
     123265-52-1P 134140-85-5P 134141-36-9P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and hydrogenation of)
ΙT
     134090-60-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction of, with (iodoacetoxy)succinimide)
                    134090-64-5P
                                   134090-67-8P
ΙT
     134090-62-3P
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     134374-31-5P
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        (prepn. of, as probe for nucleic acid hybridization)
                   134140-87-7P
IT
     134090-61-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for automated synthesis of oligonucleotides)
     134090-63-4P
                   134374-27-9P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for nucleic acid hybridization probe)
     134140-86-6P
TΤ
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn., for automated synthesis of oligonucleotides)
TΤ
     134158-63-7
     RL: RCT (Reactant)
        (reaction of, with (iodoacetoxy)succinimide)
TΤ
     39028-27-8, N-Hydroxysuccinimide iodoacetate
                                                   42014-52-8
     RL: RCT (Reactant)
        (reaction of, with deoxyuridine deriv.)
L184 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2002 ACS
     1991:409258 HCAPLUS
ΑN
     115:9258
DN
     Preparation of single stranded labelled oligonucleotides and reactive
TI
     monomers
ΙN
     Ruth, Jerry L.
PA
     Syngene, inc., USA
     U.S., 23 pp. Cont.-in-part of U.S. Ser. No. 617,094, abandoned.
SO
     CODEN: USXXAM
דת
     Patent
T.A
     English
     ICM C07H019-073
IC
     ICS C07H019-10; C07H019-173; C07H019-20
     536027000
NCL
CC
     33-9 (Carbohydrates)
     Section cross-reference(s): 6, 9
FAN.CNT 2
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                                                           DATE
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                                          US 1987-46133
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                     Α
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     US 1987-46133
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     US 1990-505032
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     US 1994-288337
                           19940810
     US 1994-336500
                           19941109
     US 1995-484028
                           19950607
OS
    MARPAT 115:9258
GI
     For diagram(s), see printed CA Issue.
AB
     The title compds. [I; B = pyrimidine or purine residue; R = linker
     attached to a blocking group, a detectable label e.g., residue of
     fluorescein or luminol or its derivs., or a solid support; when R4 =
     blocking group, then R5 = reactive phosphorus-contg. group or H if the
     5'-OH group of the 5'-terminal nucleotide of a growing oligonucleotide
     contains a reactive phosphorus-contg. group; when R5 = blocking group,
     then R4 = reactive phosphorus-contg. group or H if the 3'-OH group of the
     3'-terminal nucleotide of a growing oligonucleotide contains a reactive
     phosphorus-contg. group], useful for detection or identification of DNA by
     hybridization, are prepd. 5-[3-(Trifluoroacetamido)propenyl]-2'-
     deoxyuridine (prepn. given) was 5'-tritylated with dimethoxytrityl
     chloride and then hydrogenated to give 5'-dimethoxytrityl-5-[3-
     (trifluoroacetamido)propyl]-2'-deoxyuridine, which was condensed with
    MeOPCl2 to give 5'-dimethoxytrityl-5-[3-(trifluoroacetamido)propyl]-2'-
     deoxyuridine 3'-[methyl phosphoromonochloridite]. This was then
     incorporated into a pentadecanucleotide [II; Um = 5-(3-aminopropyl)uracil
     residue]. II [Um = 5-[2-[(7-aminoheptyl)carbamoyl]vinyl]uracil residue]
     in an aq. Na borate or Na carbonate buffer contg. NaCl was reacted with
     fluorescein isothiocyanate at 4-25.degree. overnight to give II [Um = Q,
     Q1 = fluorescein residue]. Conjugation of the prepd. I with alk.
    phosphatase is also demonstrated.
    nucleotide reporter group prepn; labeled nucleotide
ST
    DNA hybridization probe
ΙT
    Nucleic acid hybridization
        (probes for, reporter group-contg.
        oligodeoxyribonucleotides for)
TΤ
     Nucleotides, polymers
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (oligo-, deoxyribo-, labeled, prepn. of, as DNA hybridization probes)
IT
     407-25-0
     RL: RCT (Reactant)
        (acylation by, of adenosine deriv.)
IT
     93-97-0, Benzoic anhydride
     RL: RCT (Reactant)
        (acylation by, of cytidine deriv.)
IT
     96102-29-3
                 96102-32-8
     RL: RCT (Reactant)
        (acylation of)
IT
     383-65-3, N-Allyltrifluoroacetamide
     RL: RCT (Reactant)
        (alkenylation by, of uridine deriv.)
     65505-76-2 65523-09-3
IT
     RL: RCT (Reactant)
        (alkenylation of)
     70-34-8, 1-Fluoro-2, 4-dinitrobenzene
IT
     RL: RCT (Reactant)
        (condensation of, with [(aminohexyl)amino]adenine-contg.
        oligonucleotide)
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74855-51-9
                  78635-95-7
                                            78635-97-9
                                                          96102-35-1
TT
                               78635-96-8
     134128-78-2
     RL: RCT (Reactant)
        (condensation of, with nucleoside phosphites in prepn. of
        oligonucleotides)
IT
     27072-45-3, Fluorescein isothiocyanate
                                              66612-29-1
     RL: RCT (Reactant)
        (condensation of, with oligonucleotide)
                                               89992-70-1
                                                             134128-79-3
ΙT
     3279-26-3, Methyl phosphorodichloridite
     RL: RCT (Reactant)
        (condensation of, with uridine deriv.)
IT
     96102-36-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and condensation of, with fluorodinitrobenzene)
IT
     96102-22-6P 96102-24-8P
                               96102-25-9P
                                             96102-26-0P
                                               96102-35-1P
                                                              106857-10-7P
     96102-28-2P
                   96102-31-7P
                                 96102-34-0P
     134128-80-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction of, in prepn. of oligonucleotides with
        reporter groups)
                   96102-33-9P
ΙT
     96102-30-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and tritylation of)
IT
     9001-78-9DP, conjugate with reporter group-contg.
     nucleotide
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IT
     27072-45-3DP, conjugate with oligonucleotide
                                                     96118-77-3DP,
     fluoresceinaminocabonyl deriv.
                                     134090-88-3P
                                                     134090-90-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, as DNA hybridization probe)
ΙŤ
     96118-77-3P
                   96476-83-4P
                                 134090-70-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, in prepn. of labeled oligonucleotide DNA hybridization
        probes)
     40615-36-9
ΙT
     RL: RCT (Reactant)
        (tritylation by, of nucleoside derivs.)
L184 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     1987:631607 HCAPLUS
     107:231607
DN
     Base dynamics of nitroxide-labeled thymidine analogs incorporated into
TI
     (dA-dT)n by DNA polymerase I from E. coli
ΑU
     Pauly, Gary T.; Thomas, Ingrid E.; Bobst, Albert M.
     Dep. Chem., Univ. Cincinnati, Cincinnati, OH, 45221, USA
CS
SO
     Biochemistry (1987), 26(23), 7304-10
     CODEN: BICHAW; ISSN: 0006-2960
DT
     Journal
LA
     English
CC
     6-2 (General Biochemistry)
     Section cross-reference(s): 7, 9
     Nitroxide-labeled thymidine substrates (dL) for Escherichia coli DNA
ΑB
     polymerase I (pol I) were used to synthesize spin-labeled alternating
     double-stranded copolymers with (dA-dT)n as a template. All dL substrates
     use an alkane or alkene tether substituted into the 5-position of the
     pyrimidine ring to link a 5- or 6-membered ring nitroxide to the
     pyrimidine base. The kinetics of dL incorporation show some tether
     dependence with respect to tether length and tether geometry. The ESR
     spectra of (dA-dT,dL)n duplexes directly formed by polymn. with pol I are
     compared with the ESR spectra of (dA)n(dT,dL)n duplexes, which are
```

obtained after annealing of nitroxide-labeled single strands with complementary unlabeled single strands. The ESR spectra indicate that

nitroxide-labeled analogs with tethers short enough to let the nitroxide ring reside in the major groove are excellent reporter groups for monitoring hybridization. A small difference between the ESR line shapes of the alternating duplexes (dA-dT,dL) n and the homopolymer duplexes (dA)n(dT,dL)n contg. the same dL is detectable, suggesting the presence of subtle differences in the base dynamics between both systems. Computer simulation of the ESR spectra of the (dA-dT,dL)n duplexes was successful with the same motional model reported earlier. The thymidine motion arising from tilting and torsion of base pairs and base twisting in (dA-dT)n is similar to that in (dA)n(dT)n and is of the order of 4 ns.

- ST thymidine nitroxide label polynucleotide base dynamics; DNA polymerase thymidine nitroxide label
- IT Nucleic acid bases
  - RL: PRP (Properties)

(dynamics of, in polynucleotides, nitroxide-labeled thymidine analogs as probes of)

IT Conformation and Conformers

(of nucleic acid bases, in polynucleotides, dynamics of, nitroxide-labeled thymidine analogs as probes of)

IT 9012-90-2

RL: BIOL (Biological study)

(I, thymidine nitroxide analog-contg. DNAs prepn. with, for base dynamics study)

IT 111085-67-7 111186-71-1

RL: BIOL (Biological study)

(base dynamics of nitroxide-labeled thymidine analog in)

IT 111085-69-9P 111112-20-0P 111112-32-4P 111186-73-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(double-stranded, prepn. and base dynamics of nitroxide-labeled thymidine analogs in)

IT 50-89-5D, Thymidine, nitroxide-labeled derivs. 111060-17-4

111060-18-5 111085-66-6 111138-82-0

RL: RCT (Reactant)

(polymn. of, with DNA polymerase I, for use as probe of base dynamics in polynucleotides)

IT 111085-68-8P 111186-72-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and base dynamics of nitroxide-labeled thymidine analogs in)

L184 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2002 ACS

AN 1985:204247 HCAPLUS

DN 102:204247

- TI Defined sequence single strand oligonucleotides incorporating reporter groups, and nucleosides useful in such synthesis
- IN Ruth, Jerry L.
- PA Molecular Biosystems, Inc., USA
- SO PCT Int. Appl., 85 pp. CODEN: PIXXD2
- DT Patent
- LA English
- IC C07H017-00; C07H019-06; C07H015-12; C12Q001-68
- CC 33-10 (Carbohydrates)

Section cross-reference(s): 6, 9

FAN.CNT 2

FAN.CNI Z									
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE					
PI	WO 8403285	A1 19840830	WO 1984-US279	19840222 <					
	W: AU, DK,	JP, NO, US							
	RW: CH, DE,	FR, GB, NL, SE							
	AU 8428139	A1 19840910	AU 1984-28139	19840222 <					
	AU 596068	B2 19900426							

	JP	60500717	Т2	19850403		JΡ	1984-501526	19840222	<
	JP	03059914	B4	19910912					
	ΕP	135587	A1	19850403		EP	1984-901462	19840222	<
	ΕP	135587	B1	19900502					
		R: CH, DE,	FR, GB,	, LI, NL,	SE				
	CA	1231650	A1	19880119		CA	1984-460489	19840807	<
	NO	8404196	Α	19841019		NO	1984-4196	19841019	<
	NO	170890	В	19920914					
	NO	170890	С	19921223					
	DK	8405021	Α	19841219		DK	1984-5021	19841019	<
	JР	03086897	A2	19910411		JP	1990-197582	19900723	<
	JP	2542453	B2	19961009					
PRAI	US	1983-468498		19830222	<				
	WO	1983-US254		19830222	<				
	WO	1984-US279		19840222	<				
GI									

Defined sequence oligonucleotides I (n = 1-199; R = H, OH; B is any of the AΒ naturally occurring purine or pyrimidine base; the nucleotide units having naturally occurring bases are independently intermixed with one or more nucleotide units having modified bases Bm contg. the reporter groups) and the nucleosides useful in their synthesis were prepd. The oligonucleotides with the reporter groups are useful in the identification, localization and detection of complementary nucleic acid sequences of interest in cellular or cell-free systems (no data). The oligonucleotides were prepd. by coupling reaction of the appropriate units on a solid support. Thus, 5-(chloromercuri)-2'deoxyuridine was treated with N-(7-trifluoroacetylaminoheptyl)acrylamide in MeOH in the presence of Li tetrachloropalladate to give 5-[N-trifluoroacetylaminoheptyl]-1-acrylamido]-2'-deoxyuridine. latter was used in the synthesis of a pentadecadeoxynucleotide in which 5 nucleotides had 5-[N-(7-aminoheptyl)-1-acrylamido]uracil as the modified The pentadecadeoxynucleotide was treated with fluorescein isothiocyanate to give the fluoresceinated oligodeoxynucleotide. ST oligonucleotide reporter group; nucleotide oligo reporter group; fluoresceinated deoxyoligonucleotide;

(prepn. of, for synthesis of oligonucleotides incorporating

reporter groups)

IT Nucleotides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(oligo-, reporter group-contg., prepn. of)

IT 15525-45-8

RL: SPN (Synthetic preparation); PREP (Preparation)

nucleoside modified purine pyrimidine

Nucleosides, preparation

IT

```
RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for coupling of (chloromercuri)deoxyuridine with
        allyltrifluoroacetamide)
     96102-23-7
IT
     RL: RCT (Reactant)
        (coupling of, with (chloromercuri)deoxyridine)
     383-65-3
ΙŢ
     RL: RCT (Reactant)
        (coupling of, with (chloromercuri)deoxyuridine)
     65523-09-3
IT
     RL: RCT (Reactant)
        (coupling of, with allyltrifluoracetamide)
ΙT
     65505-76-2
     RL: RCT (Reactant)
        (coupling of, with allyltrifluoroacetamide)
TΤ
     74855-51-9
                  78635-95-7 78635-96-8
                                             78635-97-9
                                                          96280-61-4
     RL: RCT (Reactant)
        (nucleotide coupling reaction of, in synthesis of oligonucleotides
        incorporating reporter groups)
                   96102-33-9P
ΙT
     96102-30-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and dimethoxytritylation of)
TΤ
     96102-26-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and phosphorylation of, with methyl phosphodichloridate)
ΙT
     96118-77-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction of, with fluorescein isothiocyanate)
IT
     96102-36-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction of, with fluorodinitrobenzene)
ΙT
     96230-55-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and reaction of, with isoluminol deriv.)
     96102-27-1P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and N-benzoylation of)
ΙT
     96476-83-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     96102-22-6P 96102-24-8P
                               96102-25-9P
                                              96102-28-2P
     96102-31-7P
                   96102-34-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, in synthesis of oligonucleotides incorporating
        reporter groups)
ΙT
     96102-35-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn., in synthesis of oligonucleotides incorporating
        reporter groups)
     27072-45-3
ΤТ
     RL: RCT (Reactant)
        (reaction of, with amino group-substituted oligonucleotides)
     70-34-8
TΤ
     RL: RCT (Reactant)
        (reaction of, with aminohexyl-substituted oligodeoxynucleotide)
     66612-29-1
TΤ
     RL: RCT (Reactant)
        (reaction of, with carboxyethenyl-substituted deoxyoligonucleotide)
ΙT
     96102-32-8
     RL: RCT (Reactant)
        (trifluoroacetylation of)
IT
     96102-29-3
     RL: RCT (Reactant)
```

# (N-benzoylation of)

L184 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2002 ACS 1980:509555 HCAPLUS AN DN 93:109555 ΤI Thymidine phosphorylase. Substrate specificity for 5-substituted 2'-deoxyuridines AU Nakayama, Chikao; Wataya, Yusuke; Meyer, Rich B., Jr.; Santi, Daniel V.; Saneyoshi, Mineo; Ueda, Tohru CS Dep. Pharm. Chem., Univ. California, San Francisco, CA, 94143, USA SO J. Med. Chem. (1980), 23(8), 962-4 CODEN: JMCMAR; ISSN: 0022-2623 DT Journal LA English CC 7-3 (Enzymes) Section cross-reference(s): 1 GΙ

The title compds. I (R = halogen, Me, CF3, CN,  $\cdot$  CHO, etc.) were evaluated AΒ as substrates of horse liver thymidine phosphorylase. An improved continuous spectrophotometric assay for phosphorolysis and transferase activities of the enzyme is described. I having electron-withdrawing 5-substituents at least the size of a Me group showed lower Km, and in most cases, Vmax values. Quant. structure-activity relations relating to catalytic efficiency for various substrates to a single variable, the inductive field const., are described. ST thymidine phosphorylase specificity deoxyuridine analog; inductive field thymidine phosphorylase deoxyuridine ΙT Linear free energy relationship (of deoxyuridines, as substrates for thymidine phosphorylase) IT Michaelis constant (of thymidine phosphorylase) Molecular structure-biological activity relationship IT (enzyme-affecting, of deoxyuridine analogs) IT Linear free energy relationship (multiparameter, of deoxyuridine analogs as substrates of thymidine phosphorylase) 50-89-5, biological studies 50-90-8 50-91-9 54-42-2 IT 59-14-3 70-00-8 73-39-2 4494-26-2 5116-24-5 15176-29-1 26639-00-9 74311-81-2 RL: BIOL (Biological study)

(as substrate for thymidine phosphrylase)

IT 9030-23-3

RL: BIOL (Biological study)

(substrate specificity of, for deoxyuridine analogs, QSAR in)

=> fil reg FILE 'REGISTRY' ENTERED AT 14:17:37 ON 09 JUL 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 8 JUL 2002 HIGHEST RN 437701-77-4 DICTIONARY FILE UPDATES: 8 JUL 2002 HIGHEST RN 437701-77-4

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d ide can tot 1192

L192 ANSWER 1 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **186696-59-3** REGISTRY

CN Uridine, 5-[4-[(4-bromo-1-oxobutyl)amino]butyl]-2'-deoxy- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H26 Br N3 O6

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 2 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:353707

REFERENCE 2: 126:153646

L192 ANSWER 2 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **186696-58-2** REGISTRY

CN Uridine, 2'-deoxy-5-[4-[(iodoacetyl)amino]butyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H22 I N3 O6

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:153646

L192 ANSWER 3 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 186696-57-1 REGISTRY

CN Uridine, 5-[3-[(4-bromo-1-oxobutyl)amino]propyl]-2'-deoxy- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H24 Br N3 O6

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:153646

L192 ANSWER 4 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 171258-27-8 REGISTRY

CN Uridine, 5-[3-[[4-[4-[bis(2-chloroethyl)amino]phenyl]-1-oxobutyl]amino]propyl]-2'-deoxy- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H36 C12 N4 O6

SŘ CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:306344

REFERENCE 2: 131:154471

REFERENCE 3: 124:308654

REFERENCE 4: 124:2498

L192 ANSWER 5 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **161601-20-3** REGISTRY

CN Uridine, 2'-deoxy-5-[3-[2-[(trifluoroacetyl)amino]ethoxy]propyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H22 F3 N3 O7

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

1: 135:353707 REFERENCE

REFERENCE 2: 126:330802

REFERENCE 3: 126:153646

REFERENCE 122:178406 4:

L192 ANSWER 6 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 161601-19-0 REGISTRY

CN Uridine, 2'-deoxy-5-[3-[2-[(trifluoroacetyl)amino]ethoxy]-1-propynyl]-

(CA INDEX NAME) (9CI) FS STEREOSEARCH

MF

C16 H18 F3 N3 O7

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:353707

REFERENCE 126:330802 2:

REFERENCE 126:153646 3:

REFERENCE 4: 122:178406

L192 ANSWER 7 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 134158-63-7 REGISTRY

CN Uridine, 2'-deoxy-5-[3-[(trifluoroacetyl)amino]propyl]- (9CI) (CA INDEX NAME)

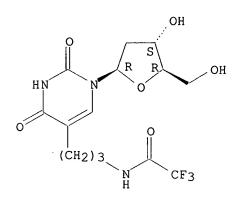
FS STEREOSEARCH

MF C14 H18 F3 N3 O6

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1967 TO DATE)

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:73170

REFERENCE 2: 132:208083

REFERENCE 3: 126:199794

REFERENCE 4: 115:9259

L192 ANSWER 8 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **134141-36-9** REGISTRY

CN Uridine, 2'-deoxy-5-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H23 N3 O7

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:353707

REFERENCE 2: 126:330802

REFERENCE 3: 126:153646

REFERENCE 4: 122:178406

REFERENCE 5: 120:127925

REFERENCE 6: 119:221156

REFERENCE 7: 115:9259

L192 ANSWER 9 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **134140-85-5** REGISTRY

CN Uridine, 2'-deoxy-5-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-butynyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H19 N3 O7

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:353707

REFERENCE 2: 126:330802

REFERENCE 3: 126:153646

REFERENCE 4: 122:178406

REFERENCE 5: 120:127925

REFERENCE 6: 119:221156

REFERENCE 7: 115:9259

L192 ANSWER 10 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **123265-52-1** REGISTRY

CN Uridine, 2'-deoxy-5-[3-[(iodoacetyl)amino]propyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C14 H20 I N3 O6

SR CA

LC STN Files: CA, CAPLUS

4 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:153646

REFERENCE 2: 119:221156

REFERENCE 3: 115:9259

REFERENCE 4: 111:190574

L192 ANSWER 11 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 96102-24-8 REGISTRY

CN Uridine, 2'-deoxy-5-[3-oxo-3-[[7-[(trifluoroacetyl)amino]heptyl]amino]-1-propenyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H29 F3 N4 O7

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:9258

REFERENCE 2: 102:204247

L192 ANSWER 12 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **96102-22-6** REGISTRY

CN Uridine, 2'-deoxy-5-[3-[(trifluoroacetyl)amino]-1-propenyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C14 H16 F3 N3 O6

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

11 REFERENCES IN FILE CA (1967 TO DATE)

11 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:131133

REFERENCE 2: 133:204750

REFERENCE 3: 130:81787

REFERENCE 4: 117:186043

REFERENCE 5: 115:9258

REFERENCE 6: 113:111963

REFERENCE 7: 106:172474

REFERENCE 8: 106:172449

REFERENCE 9: 106:81222

REFERENCE 10: 106:46883

L192 ANSWER 13 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **74311-81-2** REGISTRY

CN Uridine, 2'-deoxy-5-(1-propenyl)- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 5-(1-Propenyl)-2'-deoxyuridine

FS STEREOSEARCH

MF C12 H16 N2 O5

LC STN Files: BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAPLUS, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

7 REFERENCES IN FILE CA (1967 TO DATE)

7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:41448

REFERENCE 2: 113:224123

REFERENCE 3: 110:128633

REFERENCE 4: 103:16283

REFERENCE 5: 98:191291

REFERENCE 6: 95:7706

REFERENCE 7: 93:109555

L192 ANSWER 14 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **26639-00-9** REGISTRY

CN Uridine, 5-cyano-2'-deoxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Pyrimidinecarbonitrile, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)1,2,3,4-tetrahydro-2,4-dioxo- (8CI)

1,2,5,4-tettanydio-2,4-dioxo-

OTHER NAMES:

CN 5-Cyano-2'-deoxyuridine

CN 5-Cyanodeoxyuridine

FS STEREOSEARCH

DR 56653-12-4

MF C10 H11 N3 O5

LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAPLUS, EMBASE, TOXCENTER, USPATFULL (\*File contains numerically searchable property data)

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27 REFERENCES IN FILE CA (1967 TO DATE)
              27 REFERENCES IN FILE CAPLUS (1967 TO DATE)
            1: 136:401971
REFERENCE
                136:179979
REFERENCE
            2:
REFERENCE
            3:
                123:266
REFERENCE
                110:24209
REFERENCE
            5:
                104:28476
REFERENCE
            6:
                101:122468
REFERENCE
            7:
                100:188438
REFERENCE
                100:61328
            8:
REFERENCE
                98:209571
            9:
REFERENCE 10: 98:46574
L192 ANSWER 15 OF 20 REGISTRY COPYRIGHT 2002 ACS
    15176-29-1 REGISTRY
    Uridine, 2'-deoxy-5-ethyl- (8CI, 9CI) (CA INDEX NAME)
CN
OTHER NAMES:
     .beta.-5-Ethyl-2'-deoxyuridine
CN
     .beta.-5-Ethyldeoxyuridine
CN
CN
     2'-Deoxy-5-ethyluridine
     5-Ethyl-1-(2'-deoxy-.beta.-D-ribofuranosyl)uracil
CN
     5-Ethyl-2'-deoxyuridine
CN
     5-Ethyldeoxyuridine
ÇN
    Aedurid
CN
CN
    Edoxudine
CN
    EDU
CN
    Epoxudine
     STEREOSEARCH
FS
DR
     46895-01-6
MF
    C11 H16 N2 O5
CI
    COM
                 ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA,
LC
     STN Files:
       CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU,
       DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, NAPRALERT,
       PHAR, RTECS*, SPECINFO, TOXCENTER, USAN, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources: EINECS**, WHO
         (**Enter CHEMLIST File for up-to-date regulatory information)
```

264 REFERENCES IN FILE CA (1967 TO DATE)
17 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
264 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:272759

REFERENCE 2: 136:217007

REFERENCE 3: 136:64094

REFERENCE 4: 136:17266

REFERENCE 5: 135:376707

REFERENCE 6: 135:340189

REFERENCE 7: 135:205505

REFERENCE 8: 135:174643

REFERENCE 9: 135:116203

REFERENCE 10: 135:51041

L192 ANSWER 16 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 5116-24-5 REGISTRY

CN Thymidine, .alpha.-hydroxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Uridine, 2'-deoxy-5-(hydroxymethyl)- (6CI, 7CI, 8CI)

OTHER NAMES:

CN .alpha.-Hydroxythymidine

CN 2'-Deoxy-5-(hydroxymethyl)uridine

CN 2'-Desoxy-5-hydroxymethyluridine

CN 5-(Hydroxymethyl)-2'-desoxyuridine

CN 5-Hydroxymethyl-2'-deoxyuridine

CN 5-Hydroxymethyldeoxyuridine

FS STEREOSEARCH

MF C10 H14 N2 O6

LC STN Files: AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, CSNB, EMBASE, MEDLINE, NIOSHTIC, RTECS\*, TOXCENTER, USPATFULL (\*File contains numerically searchable property data)

Other Sources: EINECS\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

157 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

157 REFERENCES IN FILE CAPLUS (1967 TO DATE) 5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:340083

REFERENCE 2: 136:199541

REFERENCE 3: 136:5251

REFERENCE 4: 136:4440

REFERENCE 5: 135:222687

REFERENCE 6: 135:180209

REFERENCE 7: 135:135424

REFERENCE 8: 135:86583

REFERENCE 9: 134:219160

REFERENCE 10: 134:86488

L192 ANSWER 17 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 4494-26-2 REGISTRY

CN Uridine, 2'-deoxy-5-formyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Pyrimidinecarboxaldehyde, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo- (7CI, 8CI)

CN 5-Pyrimidinecarboxaldehyde, 1-(2-deoxy-.beta.-D-ribofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo- (6CI)

OTHER NAMES:

CN 2'-Deoxy-5-formyluridine

CN 5-Formyl-2'-deoxyuridine

FS STEREOSEARCH

MF C10 H12 N2 O6

LC STN Files: BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX, EMBASE, MEDLINE, RTECS\*, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

68 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

68 REFERENCES IN FILE CAPLUS (1967 TO DATE)

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:242869

REFERENCE 2: 135:315102

REFERENCE 3: 135:86583

REFERENCE 4: 135:15353

REFERENCE 5: 134:362886

REFERENCE 6: 134:321927

REFERENCE 7: 134:2074

REFERENCE 8: 133:146438

REFERENCE 9: 133:129502

REFERENCE 10: 133:116791

L192 ANSWER 18 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **73-39-2** REGISTRY

CN Uridine, 2'-deoxy-5-(2-propenyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Uridine, 5-allyl-2'-deoxy- (7CI, 8CI)

OTHER NAMES:

CN 5-Allyl-2'-deoxyuridine

CN 5-Allyldeoxyuridine

FS STEREOSEARCH

MF C12 H16 N2 O5

LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, EMBASE, MEDLINE, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

22 REFERENCES IN FILE CA (1967 TO DATE)
22 REFERENCES IN FILE CAPLUS (1967 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:144636

REFERENCE 2: 136:37859

REFERENCE 3: 133:129502

REFERENCE 4: 127:205817

REFERENCE 5: 126:182770

REFERENCE 6: 121:124571

REFERENCE 7: 116:6906

REFERENCE 8: 106:66985

REFERENCE 9: 103:196357

REFERENCE 10: 101:143556

L192 ANSWER 19 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN **70-00-8** REGISTRY

CN Thymidine, .alpha.,.alpha.,-trifluoro- (8CI, 9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN Uridine, 2'-deoxy-5-(trifluoromethyl)- (7CI)

OTHER NAMES:

CN 2'-Deoxy-5-(trifluoromethyl)uridine

CN 5-(Trifluoromethyl)-2'-deoxyuridine

CN 5-(Trifluoromethyl)deoxyuridine

CN 5-Trifluoromethyl-2'-deoxy-.beta.-uridine

CN 5-Trifluorothymidine

CN Trifluorothymidine

CN Trifluridine

CN Viroptic

FS STEREOSEARCH

MF C10 H11 F3 N2 O5

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC, PHAR, PROMT, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPATFULL, VETU

(\*File contains numerically searchable property data)
Other Sources: EINECS\*\*, WHO
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

391 REFERENCES IN FILE CA (1967 TO DATE)

20 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

391 REFERENCES IN FILE CAPLUS (1967 TO DATE)

17 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:401971

REFERENCE 2: 136:345786

REFERENCE 3: 136:252482

REFERENCE 4: 136:123678

REFERENCE 5: 136:74472

REFERENCE 6: 136:64094

REFERENCE 7: 136:37866

REFERENCE 8: 136:17266

REFERENCE 9: 136:16468

REFERENCE 10: 135:376707

L192 ANSWER 20 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 50-89-5 REGISTRY

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN .beta.-D-Ribofuranoside, thymine-1 2-deoxy-

CN 1-(2-Deoxy-.beta.-D-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione

CN 2'-Deoxythymidine

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-5-methyl-

CN 5-Methyl-2'-deoxyuridine

CN 5-Methyldeoxyuridine

CN Deoxyribothymidine

CN Deoxythymidine

CN dT

CN DThyd

```
CN Thymidin
```

CN Thymine 2-desoxyriboside

CN Thymine deoxyriboside

CN Uridine, 2'-deoxy-5-methyl-

AR 157049-39-3, 157049-40-6

FS STEREOSEARCH

DR 35902-13-7

MF C10 H14 N2 O5

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DETHERM\*, DRUGU, EMBASE, GMELIN\*, HODOC\*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK\*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPATFULL, VETU

(\*File contains numerically searchable property data)
Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

# Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6335 REFERENCES IN FILE CA (1967 TO DATE)
338 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6337 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 137:20545

REFERENCE 2: 137:17755

REFERENCE 3: 137:1836

REFERENCE 4: 136:401970

REFERENCE 5: 136:396666

REFERENCE 6: 136:395954

REFERENCE 7: 136:386335

REFERENCE 8: 136:386330

REFERENCE 9: 136:385047

REFERENCE 10: 136:384397

S√Ak

014 15

 $N\sim\sim O$ 

@16 17

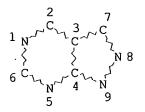
 $N \sim O \sim Ak$ 

018 19 20

=>

=>

=> d sta que 148 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 7

NUMBER OF NODES IS

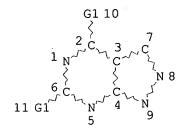
STEREO ATTRIBUTES: NONE

L45 11393 SEA FILE=REGISTRY SSS FUL L43

O√ Ak

@12 13

L46 STR



 $N \sim N$ N~^ Ak~^ N @21 22 @23 24 25

VAR G1=H/O/12/S/14/16/18/N/21/23

NODE ATTRIBUTES:

CONNECT IS M1 RC AT

CONNECT IS M1 RC AT 9

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 7

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

2557 SEA FILE=REGISTRY SUB=L45 CSS FUL L46

100.0% PROCESSED 11393 ITERATIONS

SEARCH TIME: 00.00.01

2557 ANSWERS

=> d sta que 1166

L161

## NODE ATTRIBUTES:

CONNECT IS M1 RC AT 13
CONNECT IS M1 RC AT 14
CONNECT IS M1 RC AT 16
CONNECT IS M1 RC AT 17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

# GRAPH ATTRIBUTES:

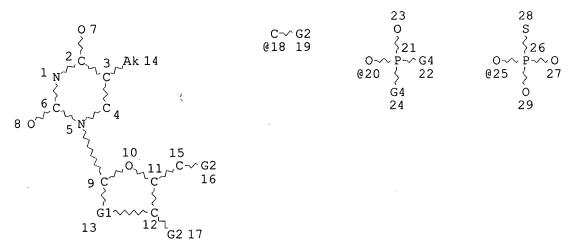
RSPEC 5

NUMBER OF NODES IS 17

### STEREO ATTRIBUTES: NONE

L163 37623 SEA FILE=REGISTRY CSS FUL L161

L164 STR



O√Ak @30 31

VAR G1=C/18 VAR G2=O/30/20/25 VAR G4=O/30 NODE ATTRIBUTES: CONNECT IS M1 RC AT 14 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 5

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

L166 2269 SEA FILE=REGISTRY SUB=L163 CSS FUL L164

100.0% PROCESSED 37623 ITERATIONS

2269 ANSWERS

SEARCH TIME: 00.00.17

#### => d his

L31

5 S L30 AND L1-L30

(FILE 'HOME' ENTERED AT 10:56:25 ON 09 JUL 2002) SET COST OFF

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FILE 'HCAPLUS' ENTERED AT 10:56:36 ON 09 JUL 2002
                E PETRIE C/AU
L1
             20 S E3, E6, E7, E11-E13
                E MEYER R/AU
            408 S E3, E7
L2
            209 S E102-E106,E110
L3
                E TBAONE J/AU
                E TABONE J/AU
             55 S E3-E6
L4
                E HURST G/AU
L5
             14 S E3, E7, E8
L6
             12 S E33-E35
L7
            707 S L1-L6
            79 S L7 AND OLIGO?
rs
            138 S L7 AND (NUCLEIC OR ?NUCLEO?)
L9
            138 S L8, L9
L10
             25 S L7 AND (?CROSSLINK? OR ?CROSS LINK?)
L11
L12
             23 S L11 AND L10
L13
             12 S L7 AND 3/SC, SX AND L11
             23 S L12, L13
L14
                E CROSSLINK/CT
                E E13+ALL
          54748 S E2+NT
L15
          45247 S E13+NT OR E14+NT OR E15+NT OR E16+NT OR E17+NT
L16
              6 S L7 AND L16
L17
L18
             23 S L14, L17
                E PETRIE C/AU
             67 S E3-E7, E10-E13
L19
L20
              7 S L19 AND (L15, L17 OR ?CROSSLINK? OR ?CROSS LINK?)
L21
              6 S L18 AND L20
              1 S L20 NOT L21
L22
L23
             23 S L18, L21
              3 S L23 AND (3H OR 125I OR 35S OR 14C OR 32P OR H3 OR I125 OR S35
L24
L25
              2 S L23 AND REPORT?
L26
              5 S L24, L25
L27
              2 S (US5824796 OR US4890348)/PN
                E US88-240474/AP, PRN
                E US89-353857/AP, PRN
L28
              5 S E4
                E US93-049807/AP, PRN
              5 S E4
L29
L30
              5 S L28, L29
```

```
5 S L27, L31 AND L1-L30
L32
L33
              3 S L26 NOT L32
L34
              8 S L32, L33
L35
             16 S L23 NOT L34.
     FILE 'REGISTRY' ENTERED AT 11:36:25 ON 09 JUL 2002
     FILE 'HCAPLUS' ENTERED AT 11:36:25 ON 09 JUL 2002
                SET SMARTSELECT ON
L36
            SEL L34 1- RN :
                                 180 TERMS
                SET SMARTSELECT OFF
     FILE 'REGISTRY' ENTERED AT 11:36:26 ON 09 JUL 2002
            180 S L36
L37
     FILE 'HCAPLUS' ENTERED AT 11:36:33 ON 09 JUL 2002
                SET SMARTSELECT ON
                                 147 TERMS
L38
            SEL L35 1- RN :
                SET SMARTSELECT OFF
     FILE 'REGISTRY' ENTERED AT 11:36:34 ON 09 JUL 2002
L39
            147 S L38
L40
            269 S L37, L39
L41
              7 S L40 AND N2C3-NCNC3/ES
             27 S L40 AND NCNC3/ES
L42
L43
                STR
L44
             50 S L43
L45
          11393 S L43 FUL
                SAV L45 OWENS693/A TEMP
L46
                STR L43
L47
             50 S L46 CSS SAM SUB=L45
L48
           2557 S L47 CSS FUL SUB=L45
                SAV L48 OWENS693A/A TEMP
L49
             71 S L48 AND I/ELS
L50
            686 S L48 AND S/ELS
L51
              0 S L50 AND (35S OR S35)
L52
            110 S L48 AND P/ELS
L53
              0 S L52 AND (32P OR P32)
L54
              1 S L48 AND (14C# OR C14#)
L55
             26 S L48 AND (3H OR H3)
L56
                STR L46
L57
              9 S L56 SAM SUB=L48
L58
            225 S L56 FUL SUB=L48
L59
                SCR 2039
L60
              0 S L59 SAM SUB=L48
              4 S L59 FUL SUB=L48
L61
                E HYDROGEN, ION/CN
L62
              3 S L48 AND (LABELED OR (D OR T)/ELS)
                E IODINE, ION/CN
L63
              1 S E116
                E SULFUR, ION/CN
L64
              1 S E144
                E CARBON, ION/CN
                E CARBON, ISOTOPE/CN
L65
              1 S E31
                E PHOSPHORUS/CN
                E PHOSPHORUS, ISOTOPE/CN
L66
              1 S E12
                E HYDROGEN, ISOTOPE/CN
L67
              1 S E6
     FILE 'HCAPLUS' ENTERED AT 11:59:07 ON 09 JUL 2002
```

L68

2817 S L48

Page 103

```
L69
          1467 S L68 AND (PY<=1988 OR PRY<=1988 OR AY<=1988)
L70
             1 S L69 AND L63-L67
L71
             80 S L69 AND (3H OR H3 OR 125I OR I125 OR 35S OR S35 OR 14C OR C14
L72
             15 S L7, L19 AND L68
L73
             8 S L72 AND L69
L74
             3 S L73 AND (LABEL? OR L71 OR ?CROSSLINK? OR ?CROSS LINK? OR REPO
L75
             67 S L69 AND (LABEL? OR ?CROSSLINK? OR ?CROSS LINK? OR REPORT?(L)G
L76
             5 S L69 AND GENET?/SC,SX
            340 S L69 AND (?OLIGO? OR ?NUCLEIC? OR ?NUCLEO?)
L77
L78
            341 S L76, L77
L79
             88 S L58
L80
             49 S L79 AND L69
             50 S L73, L80
L81
                SEL HIT RN
     FILE 'REGISTRY' ENTERED AT 12:14:53 ON 09 JUL 2002
L82
            246 S E1-E247
L83
             72 S L82 AND 46.150.18/RID
L84
            174 S L82 NOT L83
L85
            138 S L84 NOT (?CYAN? OR ?NITRIL?)/CNS
L86
            119 S L85 NOT CARBOXIMID?
L87
            118 S L86 NOT NITRO?
L88
            115 S L87 NOT NCNC2-SC4/ES
L89
            100 S L88 NOT CARBOTHI?
L90
             93 S L89 NOT BR/ELS
L91
             87 S L90 NOT ETHANAMINE
L92
             82 S L91 NOT CARBOXYLIC
L93
             78 S L92 NOT ACETIC ACID
             30 S L93 AND (C11H15N5O5 OR C10H14N6O4 OR C12H17N5O5 OR C7H8N4S2 O
L94
             4 S L94 AND C6H6N4S
L95
             3 S L95 NOT 6014-06-8
L96
L97
             4 S L94 AND C6H6N4O
L98
             1 S L97 AND 2942-47-4
             2 S L94 AND C11H14N4O5S
L100
             1 S L99 AND 76690-46-5
L101
             2 S L94 AND C11H15N5O5
L102
             1 S L101 NOT 90914-39-9
L103
             1 S L94 AND C7H8N4S2
L104
             3 S L94 AND C10H13N5O5
L105
            2 S L104 NOT 90914-38-8
L106
            2 S L94 AND C6H6N4OS
L107
             1 S L106 NOT 90914-36-6
L108
             3 S L94 AND C10H13N5O5
L109
            2 S L108 NOT 90914-38-8
L110
             3 S L94 AND C10H14N6O4
             2 S L110 NOT 90914-44-6
L111
            13 S L96, L98, L99, L102, L103, L105, L107, L109, L111
L112
            17 S L94 NOT L112
L113
             48 S L93 NOT L94
L114
L115
             77 S L85 NOT L112, L114
             8 S L115 AND (C7H10N6 OR C12H18N6O3 OR C6H15N OR C10H14N6O4 OR C1
L116
             69 S L112, L114, L116
     FILE 'HCAPLUS' ENTERED AT 13:32:14 ON 09 JUL 2002
L118
           2401 S L117
             33 S L118 AND L81
L119
             2 S L119 AND (?LABEL? OR ?FLUORES? OR REPORT?(L)GROUP? OR ?CROSSL
L120
             38 S L73, L74, L119, L120
L121
            20 S L121 AND L78
L122
L123
            18 S L121 NOT L122
L124
             1 S L122 AND DIAZO/TI
L125
             19 S L122 NOT L124
```

L167

13125 S L166

```
FILE 'HCAPLUS' ENTERED AT 13:38:35 ON 09 JUL 2002
 L126
               7 S L118 AND L7, L19
 L127
             479 S L118 AND (?OLIGO? OR GENET?/SC,SX,CW,BI OR ?NUCLEOT? OR ?NUCL
 L128
             206 S L118 AND (?LABEL? OR ?FLUORES? OR REPORT?(L)GROUP? OR ?CROSSL
            1382 S L118 AND (PY<=1988 OR PRY<=1998 OR AY<=1988)
 L129
 L130
             314 S L129 AND L127
             125 S L129 AND L128
 L131
              47 S L127 AND L128 AND L131
 L132
               2 S L132 AND L125
L133
 L134
              45 S L132 NOT L125
 L135
               7 S L134 AND OLIGO?
 L136
              6 S L135 NOT 17/SC
 L137
              8 S L133, L136
 L138
              56 S L125, L134 NOT L137
 L139
               4 S L138 AND OLIGON?
 L140
              12 S L137, L139
              52 S L138 NOT L140
L141
 L142
              23 S L141 AND NUCLE?/CW
              12 S L142 NOT (18/SC OR 9/SC OR METABOLISM/TI)
L143
              11 S L142 NOT L143
L144
                 SEL DN AN 10
               1 S L144 AND E248-E250
L145
L146
              25 S L140, L145, L143
                 SEL HIT RN
      FILE 'REGISTRY' ENTERED AT 13:49:46 ON 09 JUL 2002
             112 S E251-E362
L147
L148 .
              44 S L147 AND L117
L149
              68 S L147 NOT L148
      FILE 'HCAPLUS' ENTERED AT 13:51:19 ON 09 JUL 2002
      FILE 'HCAPLUS' ENTERED AT 13:51:44 ON 09 JUL 2002
      FILE 'REGISTRY' ENTERED AT 13:52:04 ON 09 JUL 2002
      FILE 'HCAPLUS' ENTERED AT 13:52:39 ON 09 JUL 2002
             741 S L7, L19
 L150
L151
               2 S L150 AND REPORT? GROUP?
L152
              19 S L150 AND ?LABEL?
L153
              34 S L150 AND (?FLUORES? OR DEUTER? OR TRITI?)
L154
              48 S L151, L152, L153
L155
               4 S L154 AND L68
               4 S L155 AND L1-L35, L68-L81, L118-L146, L150-L155
L156
                 SEL HIT RN
      FILE 'REGISTRY' ENTERED AT 13:55:43 ON 09 JUL 2002
L157
              11 S E363-E373
L158
               8 S L157 NOT NCNC2-SC4/ES
L159
                 STR
              50 S L159 CSS SAM
L160
                 STR L159
L161
              50 S L161 CSS SAM
L162
           37623 S L161 CSS FUL
L163
L164
                 STR L161
L165
              41 S L164 CSS SAM SUB=L163
            2269 S L164 CSS FUL SUB=L163
 L166
                 SAV OWENS693B/A L166
                 DEL OWENS693B/A
                 SAV OWENS693B/A L166 TEMP
      FILE 'HCAPLUS' ENTERED AT 14:04:57 ON 09 JUL 2002
```

```
L168
               17 S L167 AND L150
  L169
             7703 S L167 AND (PY<=1988 OR PRY<=1988 OR AY<=1988)
  L170
                5 S L168 AND L169
  L171
             2375 S L169 AND (?LABEL? OR ?FLUORE? OR DEUTER? OR TRITIUM? OR 3H OR
  L172
               86 S L169 AND (?CROSSLINK? OR ?CROSS LINK?)
  L173
               5 S L15, L16 AND L171
  L174
               88 S L170, L172, L173
  L175
              '25 S L174 AND ?OLIGON?
  L176
               78 S L174 AND (?NUCLEO? OR ?NUCLEIC?)
  L177
               7 S L174 AND GENET?/SC, SX, CW
               26 S L175, L177
  L178
  L179
               13 S L167 AND REPORT? GROUP?
               3 S L169 AND L179
  L180
  L181
               8 S L170, L180
               5 S L174 AND L181
  L182
  L183
               4 S L175, L176, L177 AND L181
  L184
                8 S L181-L183
                  SEL HIT RN
       FILE 'REGISTRY' ENTERED AT 14:09:16 ON 09 JUL 2002
               24 S E374-E397
  L185
               6 S L185 AND (C10H14N2O5 OR C11H16N2O5 OR C12H16N2O5 OR C14H18F3N
  L186
  L187
               2 S L185 AND NC4-C6/ES
      FILE 'HCAPLUS' ENTERED AT 14:13:48 ON 09 JUL 2002
                 SEL HIT RN L170
       FILE 'REGISTRY' ENTERED AT 14:14:09 ON 09 JUL 2002
  L188
              18 S E398-E415
  L189
               19 S L186, L187, L188
      FILE 'HCAPLUS' ENTERED AT 14:14:52 ON 09 JUL 2002
                  SEL HIT RN L180
      FILE 'REGISTRY' ENTERED AT 14:15:18 ON 09 JUL 2002
  L190
             7 S E416-E422
                3 S L190 NOT NC5/ES
  L191
               20 S L189, L191
  L192
      FILE 'HCAPLUS' ENTERED AT 14:16:06 ON 09 JUL 2002
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FILE 'REGISTRY' ENTERED AT 14:17:37 ON 09 JUL 2002